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Exact Bounds on Transport Coefficients

Sam Krinsky and Jerome K. Percus

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EXACT BOUNDS ON TRANSPORT COEFFICIENTS

Sam Krinsky and Jerome K. Percus

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Table of Contents

Chapter

I. Theory of Transport Coefficients and Time Correlation Functions: A Survey 1

A. Boltzmann Equation Method. 1

B. The Liouville Equation Approach 3

C. The Kubo Transform and Related Material 5

D. Kubo's Method 6

E. The Indirect Kubo Method 12

F. The Fokker-Planck Technique 13

G. The Regression Hypothesis 15

H. The Local Equilibrium Theory 18

II. The Path Integral 21

A. Introduction and Basic Formulation 21

B. Velocity Auto-Correlation 22

C. Normalization 28

D. Entropy Auto-Correlation 29

III. Imaginary Time Extension 33

A. Model of Time Extension 34

IV. Bounds upon Harmonic Oscillators

Introduction 36

A. Decoupling the Hamiltonian 36

B. Simple Inequalities 37

C. Evaluation of Sums 40

V. Comparative Perturbation Forms 44
  A. The Ordinary Anharmonic Perturbation 44
  B. Path Integral Perturbation 45
  C. Comparison of Integral Forms 47
  D. Renormalization of Terms 52
  E. Examination of Secular Coefficient 56
VI. N-Body Problem of Transport in a Debye Crystal 57
  A. Normal Mode Transformations 58
  B. Establishment of Inequalities 65
  C. N-Body Renormalization Procedure 73
VII. The Hydrodynamic Problem 78
  A. Hydrodynamic Theory of Fluctuations 78
  B. Thermodynamic Aspects of Light Scattering 82

Appendices

A. Crystal Lattice of Coupled Oscillators 87
B. Explicit Integration of Initial Velocity Dependence 90
C. N-Body Variational Equations 91
D.
  I. Typical Multiple Integrals of N-Body Calculation 94
  II. Representative Quadratic Square Forms 95
  III. N-Body Renormalization by way of Square of Frequency Shift 97
E. Path Integral Linear Terms 99
F. The Reduced Quartic Equation 100
References 103

Abstract

This work is based, in part, upon the Kubo transform technique for calculating transport coefficients by way of space-time correlation functions. These space-time correlation functions are evaluated by a special path integral formulation first described in a paper by Percus and Yevick. This integral is the basis of a minimum principle which results in bounds upon space-time correlations. The path integral representation is used to derive various auto-correlation functions, e.g. entropy-entropy; moreover, a method for representing these auto-correlations, via a minimum principle is presented. In order to establish a usable minimum principle the integrand has to be guaranteed positive definite. This is accomplished by an extension into the imaginary time domain. Thus, with analyticity in the upper half complex time plane and sufficient fall off at infinity a lower bound inequality for transport coefficients can be given.

As a simple test case the idea is applied to a model chain of oscillators and a second such system with different parameters. A simple exact inequality for the self-diffusion coefficient is obtained. A direct comparison between an ordinary perturbation expansion, to first order, for a potential of the quartic interaction type and a perturbation, to like order, in the path integral formulation, for the same interaction, is made. The two methods are seen to give the same result following a renormalization procedure. That is, the presence of certain oscillating terms in the integrand of the path integral formulation are eliminated by renormalizing, about a frequency shifted harmonic oscillator term.

Finally the path integral representation is used to discuss the N-body problem of transport in a Debye-type crystal with nearest neighbor cubic forces. To guarantee normalization, one starts with a harmonic system for which an exact solution is known and turns on the remaining quartic potential slowly from time minus infinity to time zero via a decaying exponential. The density subject to Liouville's equation has its normalization maintained since the partial time derivative of the phase-space integral of the density vanishes. One is then able at time equal to t to inquire as to the correlation of the one-body phase-space density with that at time equal to zero, allowing the calculation of transport coefficients. Specifically an inequality for the velocity-velocity correlation function is determined and its infinite imaginary time limit is examined.

CHAPTER I

Theory of Transport Coefficients and Time Correlation Functions: A Survey

Fick's law of diffusion $J_p = -D\nabla\eta$, Ohm's law of electrical condution $J_e = -\sigma\nabla\phi$ and Fourier's law of thermal conduction $q = -\lambda\nabla T$ express the generalized forces required to maintain a small steady flux of particles, charge, and heat respectively. They may also be used to describe the approach to equilibrium of a system initially in disequilibrium due to the presence of gradients in concentration η, electrostatic potential ϕ, or temperature T. The constants of proportionality are termed linear transport coefficients: diffusion D, electrical conductivity σ, thermal conductivity λ. We shall be concerned with the derivation of these transport coefficients, and their generalizations, from knowledge of the microscopic properties of the system involved. Let us first survey the approaches to this problem which have been used heretofore.

A. Boltzmann Equation Method.

The Boltzmann equation describes the nonequilibrium behavior of the single-particle distribution function of a dilute monatomic gas subject only to binary collisions. In order to obtain the transport coefficients one assumes that the system is close to local equilibrium; this is a state for which equilibrium is established in volumes which contain large numbers of particles but are still small on the scale of macroscopic variations. In each volume region one has local values of temperature T, density η, and mean velocity $\underset{\sim}{u}$. By expressing the single-particle distribution function as a local equilibrium distribution plus a correction proportional to the gradients in the local equilibrium quantities one can obtain a solvable linearized version of the Boltzmann equation. The method of solution, after Chapman and Enskog, depends upon the assumption that the single-particle distribution function is time dependent only through the time variation of the local equilibrium variables. Thus, one obtains the normal solutions presumed valid for a system close to equilibrium, and also explicit expressions for the transport coefficients. From the Boltzmann equation it is possible to generalize the macroscopic laws, e.g. Fourier's law, by considering corrections to the linearized Boltzmann equation and including nonlinear terms. Typically, Fourier's law becomes $q = -\lambda\nabla T + {}$ $+(\theta\nabla\cdot\underset{\sim}{u}\nabla T$ + other terms of like order) + higher order terms.

The method of H. Grad is to expand the distribution function in terms of Hermite polynomials, the coefficients of which are taken as state variables. The number of coefficients taken depends on the degree of approximation desired, and the complete set of Hermite coefficients is equivalent to the distribution function. If the expansion is stopped after a finite number of terms, the distribution function is obtained as a function of a number of Hermite coefficients; consequently, a determined system of differential equations can be obtained for the coefficients. By selecting a sufficient number of Hermite coefficients rather general solutions of the Boltzmannequation can be approximated.

The first systematic method for obtaining all the higher order density corrections to the Boltzmann equation was accomplished by Bogoliubov. Basic to his approach was that each higher density correction to the Boltzmann equation takes into account the interaction of more particles. However, Bogoliubov's method depends upon the functional assumption which states that the distribution functions for two or more particles do not depend explicitly upon the time. Instead, these functions depend upon time only by way of the single-particle distribution function. More recently M. S. Green gave an alternative derivation of the generalized Boltzmann equation without recourse to the functional assumption. Green's work is based upon cluster expansion methods.

B. The Liouville Equation Approach.

The method of time correlation functions is an attempt to base a linear macroscopic transport equation theory directly on the Liouville equation. The theory owes its origin to Einsten and Nyquist and of late to M. S. Green, Kubo, and Mori. The essential idea of the time correlation function method is to consider the effect of a local equilibrium state on the complete N-particle distribution function for the system. All of the obtainable information about the system is contained in the N-particle distribution function. In the time correlation function method it is assumed that the N-particle distribution function can be written as a local equilibrium N-particle distribution function plus correction terms. The local equilibrium function depends upon the local macroscopic variables, temperature, density and mean velocity and upon the position and momenta of the N particles in the system. The correction to this distribution function is determined via Liouville's equation and the assumption that at some initial time the system was in local equilibrium but at a later time is tending towards complete equilibrium. Hence, as expected, the normal solutions to Liouville's equation can be found and an expression for the corrections to local equilibrium in powers of the gradients of the local variables as well. By keeping only the first term in the gradient expansion one derives the generalized linear macroscopic transport equations. These expressions depend upon the dynamics of all N particles in the system and apply to any system, regardless of its density.

C. The Kubo Transform and Related Material.

The formulas for transport coefficients usually have the form of a one-sided Fourier transform of a time correlation function (defined as the relevant ensemble average of a two-time product A(t)B(t')).

$$(1.1) \qquad \sigma(\omega) = \int_0^\infty e^{-i\omega t} \langle \dot{A}(0)\dot{B}(t)\rangle \, dt \; .$$

The variable ω in the transform is to be regarded as a frequency and if necessary to provide convergence it can have a small imaginary part. In most cases only the low frequency behavior is of interest. At first thought it appears that in order to calculate a transport coefficient by means of time-correlations, one has to carry out the horrid task of solving the general N-body problem. However, it is really not that bad; for example, one needs only the time dependence of certain quantities $\dot{A}(p,q)$ and this information often is more accessible than the complete solution of the equations of motion.

The quantum mechanical expressions for transport coefficients are more complicated than their corresponding classical counterparts. As R. J. Zwanzig points out the following changes are to be made. (1) The functions A are replaced by their corresponding quantum mechanical operators. (2) The equilibrium phase space distribution function is replaced by the equilibrium density matrix ρ. (3) The ensemble average is calculated by taking the trace of the operator product, $<A> = \text{Trace}\,(\rho A)$. (4) The time derivative of the operator A is given by Heisenberg's equation of motion $dA/dt = i[H,A]$ where H is the system's Hamiltonian operator. The solution of this equation of motion is $A(t) = e^{itH}(A)\, e^{-itH}$. (5) Lastly, the defining relation for the time correlation function is altered by the use of the Kubo transform. The Kubo transform of an operator A is another operator $\tilde{A}$ defined by

$$\tilde{A} = \frac{1}{\beta}\int_0^\beta d\lambda\; e^{\lambda H}(A)\, e^{-\lambda H} \tag{1.2}$$

in which $\beta = 1/kT$, where k is Boltzmann's constant and T is the absolute temperature. Thus transport coefficients in quantum mechanics have the form

$$\sigma(\omega) = \int_0^\infty e^{-i\omega t} < \dot{\tilde{A}}(0)\dot{B}(t)> dt \; . \tag{1.3}$$

At sufficiently high temperatures the Kubo transform of an operator is just the operator itself and thus the quantum mechanical expressions reduce back to their classical counterparts.

D. Kubo's Method

Theoretical connections between time-correlation functions and transport coefficients have been studied from several points of view. A distinction is usually made between transport processes driven by external forces and those associated with internal forces. The response of an equilibrium system to an externally imposed force lends itself to a method after Kubo. Kubo's method is simple and operational. For instance, consider the Kubo method applied to electrical conductivity. Basically a measurement of electrical conductivity consists in the observation of the electric current responding to an applied electric field. Inasmuch as the experimental measurement is carried out repeatedly, one must average the results. The conductivity is then defined by

$$(1.4) \qquad \langle \underset{\sim}{J} \rangle = \sigma \underset{\sim}{E} + O(\underset{\sim}{E}^2)$$

where $\langle \underset{\sim}{J} \rangle$ is the average electirc current, σ the conductivity and E the applied field.

To measure the frequency dependence of the electrical conductivity one turns on a time-dependent electric field $\underset{\sim}{E}(t)$ at $t = 0$ and then measures the average current $\langle \underset{\sim}{J}(t) \rangle$. One finds

$$(1.5) \qquad \langle \underset{\sim}{J}(t) \rangle = \int_0^t dt' \, \Phi(t-t') \underset{\sim}{E}(t') + O(\underset{\sim}{E}^2)$$

where $\Phi(t-t')$ is an after-effect function showing the response at t to a disturbance at t'. One defines by Fourier analysis frequency components of the current and field,

$$(1.6) \qquad \langle \underset{\sim}{J}_\omega \rangle = \int_0^\infty e^{-i\omega t} \langle \underset{\sim}{J}(t) \rangle \, dt$$

$$\underset{\sim}{E}_\omega = \int_0^\infty e^{-i\omega t} \, \underset{\sim}{E}(t) \, dt .$$

By rearrangement one has

$$(1.7) \qquad \langle \underset{\sim}{J}_\omega \rangle = \sigma(\omega) \, \underset{\sim}{E}_\omega$$

where

$$\sigma(\omega) = \int_0^\infty e^{-i\omega t} \, \Phi(t) \, dt .$$

Kubo's statistical mechanical theory is merely a model of this experiment. As a useful aside one may derive, following Kubo, the classical response of a system due to a dynamical disturbance. The system Hamiltonian is assumed to be of the form

$$H = H_0 + H_{ext} \quad ; \qquad H_{ext} = - A \, F(t)$$

where $F(t)$ is a force and H_0 is the unperturbed Hamiltonian. The statistical distribution function of the system under discussion follows the equation of motion

$$\frac{\partial f_t}{\partial t} = - \sum \left(\frac{\partial f_t}{\partial q} \frac{\partial H_t}{\partial p} - \frac{\partial f_t}{\partial p} \frac{\partial H_t}{\partial q} \right)$$

$$= -(H_t, f_t) .$$

If the external disturbance is small the distribution function may be expressed as an unperturbed part plus a small perturbation term.

$$f_t = f + \Delta f$$

where f satisfies

$$\frac{\partial f}{\partial t} = (H,f) = 0 \quad .$$

By algebraic manipulation one determines Δf

$$\frac{\partial \Delta f}{\partial t} = (H,\Delta f) - F(t)(A,f) \quad .$$

This can be rewritten as

$$\frac{\partial \Delta f}{\partial t} = iL\Delta f - F(t)(A,f)$$

in which $iLg \equiv (H,g)$ is the Poisson bracket operator. The natural motion of any dynamical quantity A(t) is given by

$$A(t) \equiv A(P_t) = e^{-i\tau L} \; A(P_{t-\tau})$$

where P is a phase point and exp $(-i\tau L)$ represents the natural unperturbed motion of the system. This equation for A(t) is evidently a solution, corresponding to the Heisenberg picture in quantum mechanics, of

$$\frac{dA}{dt} = (A,H) \quad .$$

The solution of the Poisson bracket operator equation is

$$\Delta f(t) = \int_{-\infty}^{t} e^{i(t-t')L} \; (A,f) \; dt' \cdot F(t')$$

since $F(-\infty) = 0$, $\Delta F(-\infty) = 0$; that is, the system is in equilibrium at $t = -\infty$. The expectation value for any quantity B is

$$
\begin{aligned}
\langle \Delta B(t) \rangle &= \int B \, \Delta f(t) \, d\Gamma \\
&= - \int_{-\infty}^{t} dt' \int d\Gamma \, B \, e^{i(t-t')L} \, (A,f) \, F(t') \\
&= - \int_{-\infty}^{t} dt' \, F(t') \int (A,f) \, B(t-t') \, d\Gamma
\end{aligned}
$$

for which $d\Gamma$ is a volume element in phase-space. Thus, rewriting

$$\langle \Delta B(t) \rangle = \int_{-\infty}^{t} \Phi_{BA}(t-t') \, F(t') \, dt'$$

with the response (after-effect) function given by

$$
\begin{aligned}
\Phi_{BA}(t) &= \int (f,A) \, B(t) \, d\Gamma \\
&= \int f(A, \, B(t)) \, d\Gamma
\end{aligned}
$$

If the distribution function f is canonical

$$f = c \, e^{-\beta H}$$

and therefore,

$$(f,A) = \beta \dot{A} f$$

which finally allows one to write

$$\Phi_{BA}(t) = \beta<\dot{A}(0)B(t)>$$

$$= - \beta<A(0)\ \dot{B}(t)>$$

since $\frac{d}{dt} <A(t),\ B(t+\tau)> = 0$.

Returning to the model conductivity experiment it can, in like manner, be shown [17] that

$$(1.8) \qquad \Phi_{ba}(t) = \beta<\tilde{J}_a J_b(t)>$$

in which Φ_{ba} is the after-effect function giving, in this case, the current in the b-th direction due to a field in the a-th direction and thus $\Phi(t)$ is a time correlation function. The corresponding frequency dependent electric conductivity tensor is

$$(1.9) \qquad \sigma_{ba}(\omega) = \beta \int_0^\infty e^{-i\omega t}\ <\tilde{J}_a J_b(t)>\ dt\ .$$

Transport coefficients associated with internal disturbances e.g. thermodynamics can't be handled directly by Kubo's formulation; nevertheless, other approaches do exist and among them are the indirect Kubo method, the Fokker-Planck technique, the regression hypothesis and local equilibrium theory. Each of these approaches will be briefly reviewed.

E. The Indirect Kubo Method.

In order to clarify the indirect Kubo method a hydrodynamic problem will be discussed. At $t = 0$ an external force $\underset{\sim}{F}(\underset{\sim}{R},t)$ is applied to a fluid in thermal equilibrium. This force causes fluid motion and gives rise to a velocity field $\underset{\sim}{v}(\underset{\sim}{R},t)$. Expressing the relation between force and response as Fourier components one has

$$\begin{aligned} \underset{\sim}{F}(\omega,\underset{\sim}{k}) &= \iint \underset{\sim}{F}(\underset{\sim}{R},t)\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{R}+i\omega t}\, dt\, d^3R \\ \underset{\sim}{v}(\omega,\underset{\sim}{k}) &= \iint \underset{\sim}{v}(\underset{\sim}{R},t)\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{R}+i\omega t}\, dt\, d^3R \ . \end{aligned} \tag{1.10}$$

The solution[†] of the hydrodynamic equations of motion if the force is transverse i.e. $\nabla\cdot\underset{\sim}{F} = 0$ and $\nabla\times F \neq 0$ leads to

$$\underset{\sim}{v}(\omega,\underset{\sim}{k}) = \sigma(\omega,\underset{\sim}{k})\ \underset{\sim}{F}(\omega,\underset{\sim}{k}) \tag{1.11}$$

a transverse velocity field. Hence the coefficient $\sigma(\omega,k)$ [††] is

$$\sigma(\omega,k) = [\eta k^2 - i\omega\rho]^{-1} \ , \tag{1.12}$$

[†] for forces small enough so that the equations of motion may be linearized in deviations from equilibrium.

[††] the calculation which leads to this equation is macroscopic and follows entirely from the Navier-Stokes equation which is discussed briefly in Chapter VII.

where ρ is the mass density, and η the shear viscosity coefficient. To obtain the shear viscosity coefficient from σ(ω,k) one goes to the limit of long wavelength viz. k → 0 and then to the limit of low frequency:

$$\eta = \lim_{\omega\to 0}\lim_{k\to 0} \frac{\rho^2\omega^2}{k^2} \operatorname{Re} \sigma(\omega,k) \ . \tag{1.13}$$

However, σ(ω,k) can be obtained from Kubo's method since the force $\underset{\sim}{F}(\underset{\sim}{R},t)$ is externally applied and $\underset{\sim}{v}(\underset{\sim}{R},t)$ is a response to that force. Hence, Kubo's method leads to a statistical mechanical formula for σ(ω,k) and consequently η as well.

F. The Fokker-Planck Technique.

The Fokker-Planck theory is based upon ideas like those occurring in Brownian motion, assuming that the motion is determined by a large number of small impulses. Let $P(\underset{\sim}{R}_0, t_0/R, t)$ be the probability per unit volume of finding the particle at position R at time t, given its position R_0 at initial time t_0. This function $P(\underset{\sim}{R}_0, t_0/R, t)$ is determined by way of the Fokker-Planck equation [10]

$$\frac{\partial P}{\partial t} = \nabla\cdot(\underset{\sim}{A}P) + \nabla^2(DP) \ . \tag{1.14}$$

To interpret A and D let $\Delta\underset{\sim}{R}$ be the displacement of the particle during a time interval Δt which is small in a macroscopic sense but larger than characteric molecular times;[†]

[†] the duration of a molecular collision is of the order of 10^{-12} seconds.

then one finds in deriving the Fokker-Planck equation that $\underset{\sim}{A}$ is an average velocity,

$$(1.15) \qquad A = \lim_{\Delta t \to 0} \frac{<\Delta R>}{\Delta t}$$

and that

$$(1.16) \qquad D = \lim_{\Delta t \to 0} \frac{<(\Delta R)^2>}{6\Delta t}$$

The formula given for D, the coefficient of self-diffusion, was originally deduced by Einstein. Hence, we have in principle a method of obtaining a transport coefficient by the use of a time correlation function. If one writes the displacement of the particle as the time integral of the velocity

$$(1.17) \qquad \Delta R = \int_0^{\Delta t} v(\ell)\, d\ell$$

then D is given by

$$(1.18) \qquad D = \lim_{\Delta t \to 0} \frac{1}{6\Delta t} \int_0^{\Delta t} \int_0^{\Delta t} <v(\ell) \cdot v(\ell')>\, d\ell\, d\ell'$$

where the integrand contains the auto-correlation function of the particle velocity. By translation in time invariance one may write

$$(1.19) \qquad <v(\ell) \cdot v(\ell')> = <v(0) \cdot v(\ell'-\ell)>$$

and thus integrating one gets

$$(1.20) \qquad D = \lim_{\Delta t \to 0} \frac{1}{3} \int_0^{\Delta t} (1- \frac{\ell}{\Delta t})\, <v(0) \cdot v(\ell)>\, d\ell\ .$$

The term $\ell/\Delta t$ may be left out provided Δt is small but nonetheless macroscopic, and if the auto-correlation function decays fast enough:

$$D \simeq \frac{1}{3}\int_0^{\Delta t} \langle v(0)\cdot v(\ell)\rangle \, d\ell \,. \tag{1.21}$$

G. The Regression Hypothesis.

This method is based upon Onsager's hypothesis concerning the regression of fluctuations. The hypothesis states that spontaneous fluctuations from thermal equilibrium decay, on the average, according to the macroscopic transport laws. Kubo, Yokota, and Nakajima proposed a method based upon this hypothesis. This is illustrated as follows. Consider the macroscopic transport law concerning the average value $\bar{a}(t)$ of a dynamical quantity $a(t)$,

$$\frac{d\bar{a}(t)}{dt} = -\, M\, \bar{a}(t) \tag{1.22}$$

where clearly M is a rate constant i.e. transport coefficient for the decay of $\bar{a}(t)$. Multiply both sides of the transport law by the initial value $a(0)$, and then average over an equilibrium ensemble of initial values obtaining

$$\langle \frac{d}{dt}\, \bar{a}(t)\; a(0)\rangle = -\, M\langle \bar{a}(t)\; a(0)\rangle \,. \tag{1.23}$$

If $a(t)$ is the numerical value of a function $A(p(t),q(t))$ in phase-space, then one may write the average in the form of a time-correlation function,

$$<\bar{a}(t)a(0)> = <A(p(t),q(t))\ A(p(0),q(0))> \tag{1.24}$$
$$= <A(t)A(0)> \quad .$$

The regression hypothesis has been used implicitly. That is, in averaging over an equilibrium distribution of initial a(0), the major contribution comes from small values of a(0), on the order of spontaneous fluctuations, but one wants the transport laws to be valid for just such small initial values.

Following the above equations one may write the transport law as

$$<\dot{A}(t)A(0)> = -\ M<A(t)A(0)> \tag{1.25}$$

Integrating this equation over the small time interval (0,t)

$$\int_0^t <\dot{A}(t')A(0)>\ dt' = -\ M \int_0^t <A(t')A(0)>\ dt' \tag{1.26}$$

and if $Mt << 1$ then one obtains

$$\int_0^t <\dot{A}(t')A(0)>dt' = -Mt<A(0)A(0)>+\ O(M^2t^2)\ . \tag{1.27}$$

Using time invariance to shift the time origin i.e.

$$<\dot{A}(t')A(0)> = <\dot{A}(0)A(-t')> \tag{1.28}$$

and introducting another time derivative

(1.29) $$A(-t') = A(0) - \int_0^{t'} \dot{A}(-\ell)\, d\ell$$

gives for t small,

(1.30) $$\int_0^t \langle \dot{A}(0)A(0)\rangle dt' - \int_0^t \int_0^{t'} \langle \dot{A}(0)\dot{A}(-\ell)\rangle d\ell\, dt' = -Mt\langle A(0)A(0)\rangle \quad .$$

The first term on the left vanishes since $\langle \dot{A}A\rangle = \langle \frac{1}{2}\frac{dA^2}{dt}\rangle$ viz. the equilibrium average of a rate of change must vanish. In the second term the time origin is shifted back by an interval ℓ thus replacing $\langle \dot{A}(0)\dot{A}(-\ell)\rangle$ by $\langle \dot{A}(\ell)\dot{A}(0)\rangle$ and lastly the order of integration is reversed. Hence, performing the t' integration and dividing both sides of the equation by t gives,

(1.31) $$\int_0^t (1 - \frac{\ell}{t})\, \langle \dot{A}(\ell)\dot{A}(0)\rangle\, dt = M\langle A^2\rangle \quad .$$

Provided that the time correlation decays fast enough one may in analogy with the Fokker-Planck technique drop the ℓ/t factor and obtain

(1.32) $$M = \int_0^{\tau} \langle \dot{A}(\ell)\dot{A}(0)\rangle \,/\, \langle A^2\rangle\, d\ell$$

where the upper limit has been replaced by a time τ long enough for the integrand to have decayed to zero.

H. The Local Equilibrium Theory

This method was devised by Mori and the basis of it is the observation that when a typical nonequilibrium system relaxes toward thermal equilibrium it passes through a series of local equilibrium states. Consider the case where only a single macroscopic variable A is of interest. The ensemble mean value of this quantity is denoted by $\bar{A}$. In an equilibrium ensemble where $\bar{A}$ is held fixed by some kind of external constraint, the phase-space distribution function f(p,q) is

$$(1.33) \qquad f(p,q) = \frac{e^{-\beta H-\gamma A}}{Q}$$

where the partition function $Q(\beta,\gamma)$

$$(1.34) \qquad Q(\beta,\gamma) = \int\int e^{-\beta H-\gamma A}\, dp\, dq$$

is the normalizing factor and H is the system Hamiltonian.

This distribution function gives maximum entropy under the constraints of fixed $\bar{H}$ and $\bar{A}$. The normal thermal equilibrium distribution function, appropriate when $\bar{A}$ is not constrained, is obtained by setting $\gamma = 0$. The relationship between the Lagrange multipliers β and γ, and the mean values $\bar{H}$ and $\bar{A}$ is given by

$$(1.35) \qquad \bar{H} = -\frac{\partial \log Q}{\partial \beta} \; ; \qquad \bar{A} = -\frac{\partial \log Q}{\partial \gamma} \; .$$

The main assumption of the local equilibrium theory is that the phase-space distribution function maintains the above form for all times. However, the assumption is not correct, except in the trivial case where A like H is a constant of motion. Moreover, it has the additional failing that the mean value of the rate of change of A vanishes.

Nevertheless, the true distribution function of a relaxing system probably doesn't deviate appreciably from the locally canonical form and therefore the ideas of local equilibrium theory are used in practice. One allows a system to grow old for a certain time interval τ which is long compared to molecular collision times but short enough such that the macroscopic state of the system hasn't altered drastically. Then the mean value of the curret $J = \dot{A}$ is measured at τ. The average is

$$(1.36) \qquad \bar{J}(T) = Q^{-1} \int\int \dot{A}(\tau)\, e^{-\beta H - \gamma A}\, dp\, dq \; .$$

Small deviations from equilibrium correspond to small γ, and the thermodynamic force associated with $\bar{A}$ is

$$(1.37) \qquad F = k\gamma + O(\gamma^2)$$

where k is the usual Boltzmann constant. One then expands the average current in powers of γ

$$(1.38)\ \bar{J}(\tau) = \langle J(\tau)\rangle - \gamma\langle \dot{A}(\tau)A(0)\rangle + \gamma\langle J(\tau)\rangle\langle A(0)\rangle + O(\gamma^2)$$

and since $\langle J(\tau)\rangle$ is the current at thermal equilibrium it vanishes, so that

$$(1.39) \qquad \bar{J}(\tau) = -\,\gamma\langle \dot{A}(\tau)A(0)\rangle + O(\gamma^2) \; .$$

Following the manipulative procedure of the already outlined regression hypothesis, equation (1.39) becomes

$$\bar{J}(\tau) = L\ F(0) \tag{1.40}$$

where the transport coefficient L is given by

$$L = \frac{1}{k} \int_0^\tau <\dot{A}(\ell)\dot{A}(0)>\, d\ell \tag{1.41}$$

The various methods reviewed all lead to the same results with the following reservation. Some methods lead immediately to expressions for transport coefficients involving integrations over characteristic time intervals τ, long compared with molecular times, and short compared with macroscopic times. Other methods lead to integrals over an infinite time interval together with some limiting process (e.g. $\omega \to 0$). For all practical purposes, even though different formally, these two basic approaches should be considered identical.

CHAPTER II

A. Introduction and Basic Formulation

In equilibrium statistical mechanics all of the thermodynamic averages of a system are known if its partition function in an external field can be calculated. Similarly for the space-time correlations required in the theory of transport processes, it is possible to introduce a special time-dependent field and a time-dependent partition function to achieve the same effect. By adding a time-dependent inhomogeneous term to be described one may define the time-dependent partition function as the complete phase-space integral of a suitable N-body many time Boltzmann factor, $Z = \int G(\underset{\sim}{x},\underset{\sim}{p}) \prod_{t'=0}^{t} d\underset{\sim}{x}(t')\, d\underset{\sim}{p}(t')$ (where $\underset{\sim}{x}(t')$ and $\underset{\sim}{p}(t')$ are the possible positions and momenta for any time interval between 0 and t). To obtain the weight function for expectations which involve any $\underset{\sim}{x}(\tau)$ and $\underset{\sim}{p}(\tau)$ $(0 \leq \tau \leq t)$, one must guarantee that $\underset{\sim}{x}(\tau)$ and $\underset{\sim}{p}(\tau)$ be restricted by the equations of motion and initial conditions. Now the equations of motion can be guaranteed by applying the appropriate delta functions; whereupon,

$$(2.1)\quad G(\underset{\sim}{x},\underset{\sim}{p}|0,t) = \prod_{\tau=0}^{t} \delta(\dot{\underset{\sim}{x}}(\tau) - \frac{1}{m}\, \underset{\sim}{p}(\tau))\,\delta(\dot{\underset{\sim}{p}}(\tau) + \frac{\partial v(\tau)}{\partial \underset{\sim}{x}})\, G[\underset{\sim}{x}(0),\underset{\sim}{p}(0)]$$

for which $G[\underset{\sim}{x}(0),\underset{\sim}{p}(0)]$ is the initial unnormalized distribution usually to be taken as an equilibrium Boltzmann factor.

After Fourier representation of the delta functions, one obtains as the required generalization (to within normalization) the path integral [18]

$$G(\underset{\sim}{x},\underset{\sim}{p}|0,t) = \int \exp \left[i \int_0^t (\dot{\underset{\sim}{x}}(\tau) - \frac{1}{m}\, \underset{\sim}{p}(\tau))\cdot\underset{\sim}{\xi}(\tau)\, d\tau\right]$$

$$\tag{2.2} \cdot\exp\left[i \int_0^t (\dot{\underset{\sim}{p}}(\tau) + \frac{\partial V(\tau)}{\partial \underset{\sim}{x}})\cdot\underset{\sim}{\eta}(\tau)\, d\tau\right]$$

$$\cdot\; D\{\xi(\tau)\}\; D\{\eta(\tau)\}\; G[\underset{\sim}{x}(0),\underset{\sim}{p}(0)] \quad .$$

This is to be the basis of a variational principle and in fact a minimum principle resulting in bounds upon space-time correlations. As prototype, we consider the case of a simple harmonic oscillator. The path integral representation will be used to derive the one-body, one-dimensional velocity and entropy auto-correlation functions. In addition, a method for normalizing this simple problem will be presented.

B. Velocity Auto-Correlation for Simple Harmonic Oscillator

Before considering the path integral for this one-body example a correctly normalized expression for the velocity auto-correlation will be derived by using a simple phase-space integral. The harmonic oscillator solution in terms of initial values is

$$x(t) = x(0) \cos \omega_0 t + \frac{\dot{x}(0)}{\omega_0} \sin \omega_0 t$$

where the phase-space density is

$$\rho(x(0),\dot{x}(0)) = \frac{\beta m\omega_0}{2\pi} e^{-\frac{\beta m}{2}(\dot{x}^2(0)+\omega_0^2x^2(0))}$$

subject to $\int \rho(x(0),\dot{x}(0))\, d\dot{x}(0)\, dx(0) = 1.$

Therefore one may write

$$(2.3)\quad \langle e^{-\frac{R}{2}x(t)x(0)}\rangle = \frac{\beta m\omega_0}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{1}{2}R(x^2(0)\cos\omega_0t + \frac{x(0)\dot{x}(0)}{\omega_0}\sin\omega_0t)}\, e^{-\frac{\beta m}{2}(\dot{x}^2(0)+\omega_0^2x^2(0))}\, d\dot{x}(0)\, dx(0)$$

After integrating and differentiating with respect to R at R = 0 one obtains

$$(2.4)\qquad \langle x(t)x(0)\rangle = \frac{1}{\beta m\omega_0^2}\cos\omega_0t\ .$$

For time translational invariant systems

$$\begin{aligned}\langle\dot{x}(t)\dot{x}(0)\rangle &= \langle\dot{x}(t+t')\dot{x}(t')\rangle\\ &= -\langle\ddot{x}(t+t')x(t')\rangle \text{ by parts integration}\\ &= -\langle\ddot{x}(t)x(0)\rangle \qquad \text{as } t'\to 0\\ &= -\frac{\partial^2}{\partial t^2}\langle x(t)x(0)\rangle\end{aligned}$$

and therefore

$$(2.5)\qquad \langle\dot{x}(t)\dot{x}(0)\rangle = \frac{1}{\beta m}\cos\omega_0t$$

Returning to the unnormalized path integral representation one has in one-dimensional form

$$<G(x(t),x(0),\dot{x}(t),\dot{x}(0))>=\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} G(x(t),x(0),\dot{x}(t),\dot{x}(0))$$

$$\cdot e^{-\frac{1}{2}m\beta\dot{x}^2(0)}\, e^{-\beta\phi(x(0))}\, e^{i\int_0^t \xi(t')[\dot{x}(t')-\dot{x}(0)-\frac{1}{m}\int_0^{t'} F(x(t''))dt'']dt'}$$

$$\cdot \prod_0^t d\xi(t') \prod_{0+}^{t-} dx(t')\, dx(0)\, dx(t)\, d\dot{x}(0) \;,$$

where the initial velocity distribution has been taken as Gaussian and

$$G = e^{-\frac{1}{2}R\dot{x}(t)\dot{x}(0)}$$

with

$$\phi(x(0)) = \frac{1}{2}\, m\omega_0^2 x^2(0)$$

$$F(x(t'')) = -\, m\omega_0^2 x(t'')$$

then once again the problem is to determine

$$<\dot{x}(t)\dot{x}(0)> = -\,2\,\frac{\partial}{\partial R}\,<e^{-\frac{1}{2}R\,\dot{x}(t)\dot{x}(0)}>\Big|_{R=0} \;.$$

By integrating out the $\dot{x}(0)$ [†] dependence we get

[†] See Appendix B.

$$<e^{-\frac{1}{2}R\dot{x}(t)\dot{x}(0)}> = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-\frac{1}{2}m\beta\omega_0^2x^2(0)}$$

$$\cdot\exp - \frac{1}{2m\beta}\left[\int\int_0^t \xi(t')\xi(t'')\, dt'\, dt'' - iR\dot{x}(t)\int_0^t \xi(t')\, dt' \right.$$

$$(2.6) \qquad \left. - \frac{1}{4}R^2\dot{x}^2(t)\right] \cdot e^{i\int_0^t \xi(t')\dot{x}(t')dt'}$$

$$\cdot\, e^{i\int_0^t\int_0^{t'} \omega_0^2\xi(t')x(t'')\, dt'\, dt''} \qquad D[\ \ldots] \quad .$$

For a Gaussian integral, the steepest descent method is identical with the exact result. Hence the only problem is to find the saddle "point" (function) of the exponent. If the kernel of (2.6) is varied with respect to $\xi(\tau)$ and $x(\tau)$ (with $\tau = t',t''$) one obtains the integro-differential equations

$$(2.7) \qquad - \frac{1}{m\beta}\int_0^t \xi(t')\, dt' + \frac{iR\dot{x}(t)}{2m\beta} + i\dot{x}(\tau) + i\int_0^\tau \omega_0^2x(t'')\, dt'' = 0$$

$$(2.8) \qquad - i\,\dot{\xi}(\tau) + i\int_\tau^t \omega_0^2\,\xi(t')\, dt' = 0$$

τ-differentiating these equations and re-substituting the results gives

$\dot{\xi}(t) = 0$ a boundary condition, and

$\dot{\xi}(0) = i\beta m\omega_0^2\dot{x}(0)$ which is a coupling condition between equation sets.

The results of the τ-differentiation are

$$\ddot{x}(\tau)-\omega_0^2 x(\tau) = 0 \quad \text{subject to } x(0) = x(0);\ x(t) = x(t)$$

and

$$\ddot{\xi}(\tau) - \omega_0^2\, \xi(\tau) = 0 \ .$$

Therefore, solving these equations subject to all four conditions yields

$$x(\tau) = \frac{x(t)\sin\omega_0\tau + x(0)\sin\omega_0(t-\tau)}{\sin\omega_0 t} \tag{2.9}$$

$$\begin{aligned}\xi(\tau) &= i\beta m\omega_0^2\left(\frac{x(t)-x(0)\cos\omega_0 t}{\sin^2\omega_0 t}\right)\cos\omega_0(t-\tau)\\ &+ \frac{iR\omega_0^2}{2}\left(\frac{x(t)\cos\omega_0 t - x(0)}{\sin^2\omega_0 t}\right)\cos\omega_0(t-\tau)\ .\end{aligned} \tag{2.10}$$

Furthermore the kernel can be simplified if equation (2.7) is multiplied by $\xi(\tau)$ and integrated. In like fashion (2.8) is multiplied by $x(\tau)$ and also integrated. There results

$$\begin{aligned}&-\frac{1}{m\beta}\int_0^t\int \xi(\tau)\xi(t')\,dt'\,d\tau + i\int_0^t \xi(\tau)\dot{x}(\tau)\,d\tau\\ &+\frac{iR}{2m\beta}\int_0^t \xi(\tau)\dot{x}(t)\,d\tau + i\int_0^t\int_0^\tau \omega_0^2\,\xi(\tau)x(t'')\,dt''\,d\tau = 0\end{aligned} \tag{2.11}$$

$$(2.12) \quad - i \int_0^t \dot{\xi}(\tau)x(\tau)\,d\tau + i \int_0^t \int_\tau^t \omega_0^2\, \xi(t')x(\tau)\,dt'\,d\tau = 0 \;.$$

Integrating the single integral in (2.12) by parts and adding this result to (2.11) implies

$$\xi(t)x(t) - \xi(0)x(0) = - \frac{1}{m\beta} \int_0^t \int_0^t \xi(\tau)\xi(t')\,dt'\,d\tau$$

$$(2.13) \quad + \frac{iR}{2m\beta} \int_0^t \xi(\tau)\dot{x}(t)\,d\tau + i \int_0^t \int_0^\tau \omega_0^2\, \xi(\tau)x(t'')\,dt''\,d\tau$$

$$+ i \int_0^t \int_\tau^t \omega_0^2\, \xi(t')x(\tau)\,dt'\,d\tau + 2i \int_0^t \xi(\tau)\dot{x}(\tau)\,d\tau \;.$$

Thus the kernel is

$$e^{- \frac{1}{2} m\beta\omega_0^2 x^2(0)}\; e^{\frac{iR}{4m\beta} \dot{x}(t) \int_0^t \xi(t')dt'}\; e^{- \frac{1}{2m\beta}(- \frac{R^2}{4} \dot{x}^2(t))}$$

$$\cdot\; e^{\frac{1}{2} i(\xi(t)x(t)-\xi(0)x(0))} \;.$$

Therefore equation (2.6) becomes

$$<e^{- \frac{1}{2} R\dot{x}(t)\dot{x}(0)}> \;=\; \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{- \frac{1}{2} m\beta\omega_0^2 x^2(0)}\; e^{\frac{iR}{4m\beta}\dot{x}(t)\int_0^t \xi(t')dt'}$$

$$\cdot\; e^{\frac{R^2}{8m\beta} \dot{x}^2(t)}\; e^{\frac{1}{2} i(\xi(t)x(t)-\xi(0)x(0))} \quad dx(0)\; dx(t) \;,$$

which with the explicit reintroduction of equations (2.9) and (2.10) and some simple algebraic manipulations becomes

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp - \tfrac{1}{2}(c_{11}x^2(0)+2c_{12}x(0)x(t) \tag{2.14}$$

$$+ c_{22}x^2(t))\, dx(0)\, dx(t)$$

where

$$c_{11} = c_{22} = \frac{\beta m\omega_0^2+R\omega_0^2 \cos \omega_0 t}{\sin^2\omega_0 t}$$

$$c_{12} = -\frac{\beta m\omega_0^2 \cos \omega_0 t}{\sin^2\omega_0 t} - \frac{R\omega_0^2(1+ \cos^2\omega_0 t)}{2 \sin^2\omega_0 t} .$$

Simultaneously integrating this quadratic square and differentiating with respect to R evaluated at R = 0 yields to within normalization

$$<\dot{x}(t)\dot{x}(0)> = \frac{2\pi}{(m\beta\omega_0^2)^2}\, \omega_0^2 \cos \omega_0 t \sin \omega_0 t . \tag{2.15}$$

C. Normalization.

The normalization for expression (2.6) is

$$N = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} e^{-\frac{1}{2} m\beta\dot{x}^2(0)}\, e^{-\frac{1}{2} m\beta\omega_0^2x^2(0)}$$

$$\cdot\exp \left[i \int_0^t \xi(t')(\dot{x}(t')-\dot{x}(0) + \int_0^{t'} \omega_0^2x(t'')dt'')dt'\right] \tag{2.16}$$

$$\cdot\prod_0^t d\xi(t') \prod_0^t dx(t')\, d\dot{x}(0) ,$$

which after the variations are carried through becomes

$$N = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{1}{2}m\beta\omega_0^2 x^2(0)}$$

(2.17)
$$\cdot\ e^{-\frac{1}{2}m\beta\omega_0^2\left[\frac{x^2(t)-2x(0)x(t)\cos\omega_0 t}{\sin^2\omega_0 t}+\frac{x^2(0)\cos^2\omega_0 t}{\sin^2\omega_0 t}\right]}$$

$$dx(0)\ dx(t)$$

integrating

$$N = \frac{2\pi}{\beta m\omega_0^2}\sin\omega_0 t\ . \tag{2.18}$$

If expression (2.15) is now divided by (2.18) we get

$$\langle\dot{x}(t)\dot{x}(0)\rangle = \frac{1}{\beta m}\cos\omega_0 t\ ,$$

which is clearly identical to (2.5). Aside from the fact that this method gives the correct result its drawback is that the variational principle must be applied separately to both the expectation of a function and its purported normalization. However, this objection will be overcome in the full N-body problem by an initial normalization technique.

D. Entropy Auto-Correlation.

The entropy in a local equilibrium ensemble is defined by

$$S(t) = \frac{d}{dt}\sum_j (H_j-h_j)x_j$$

where

H_j = contribution of the j-th molecule to the Hamiltonian

h_j = enthalpy per molecule

x_j = position of j-th molecule.

For simplicity in the calculation we consider only the kinetic energy contribution to the entropy and so

$$S(t) = \frac{d}{dt}\,\frac{1}{2}\,m\dot{x}^2(t)x(t)$$

$$\equiv \frac{d}{dt}\,J(t)\ .$$

Because of time translation invariance the auto-correlation may be expressed as

$$<S(0)S(t)> = -\frac{\partial^2}{\partial t^2}<J(0)J(t)>$$

$$= -\frac{\partial^2}{\partial t^2}<\frac{1}{2}\,m\dot{x}^2(0)x(0)\ \frac{1}{2}\,m\dot{x}^2(t)x(t)>.$$

If one chooses

$$G = \frac{m^2}{4}\,\dot{x}^2(0)\ e^{-R\ x(0)\dot{x}^2(t)x(t)}$$

then as expected

$$<S(0)S(t)> = \frac{\partial^2}{\partial t^2}\frac{\partial}{\partial R}<\frac{m^2}{4}\,\dot{x}^2(0)\ e^{-R\ x(0)\dot{x}^2(t)x(t)}>\Big|_{R=0}$$

$$= -\frac{\partial^2}{\partial t^2}<\frac{m^2}{4}\,\dot{x}^2(0)x(0)\dot{x}^2(t)x(t)>\ .$$

Thus, one has

$$<G(x(t),x(0),\dot{x}(t),\dot{x}(0))>= \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\frac{m^2}{4}\,\dot{x}^2(0)$$

$$\cdot e^{-Rx(0)\dot{x}^2(t)x(t)}\ e^{-\frac{1}{2}\,m\beta\dot{x}^2(0)}\ e^{-\frac{1}{2}\,m\beta\omega_0^2x^2(0)}$$

$$\cdot e^{i\int_0^t \xi(t')[\dot{x}(t')-\dot{x}(0)+\int_0^{t'}\omega_0^2x(t'')dt'']dt'}\ D[\ldots]\ ,$$

which upon completing the square in $\dot{x}(0)$ and integrating is

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\left(\frac{1}{m\beta}-\left[\frac{1}{m\beta}\int_0^t \xi(t')\,dt'\right]^2\right)\frac{m^2}{4}\,e^{-Rx(0)\dot{x}^2(t)x(t)}$$

$$\exp\left[-\frac{1}{2}m\beta\omega_0^2x^2(0)-\frac{1}{2m\beta}\int_0^t\!\!\int \xi(t')\xi(t'')dt'\,dt''\right.$$

(2.20)

$$\left.+\,i\int_0^t \xi(t')\dot{x}(t')dt' + i\int_0^t\!\!\int_0^{t'} \omega_0^2\xi(t')x(t'')dt'\,dt''\right]$$

$$\cdot\prod_0^t d\xi(t')\prod_{0+}^{t-} dx(t')\;dx(0)\;dx(t)\;.$$

Using the same techniques as in expressions (2.6) to (2.13) we obtain

$$\langle G(x(t),\ldots)\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{1}{m\beta}-\left[\frac{1}{m\beta}\int_0^t \xi(t')\,dt'\right]^2\right)$$

(2.21)

$$\cdot\,\frac{m^2}{4}\,e^{-Rx(0)\dot{x}^2(t)x(t)}\;e^{-\frac{1}{2}m\beta\omega_0^2x^2(0)}$$

$$\cdot\, e^{\frac{1}{2}i[\xi(t)x(t)-\xi(0)x(0)]}\;dx(0)\;dx(t)$$

where $x(\tau)$ is given by (2.9) and

$$\xi(t)x(t)-\xi(0)x(0) = i\beta m\omega_0^2\left[\frac{x^2(t)-2x(0)x(t)\cos\omega_0t+x^2(0)\cos^2\omega_0t}{\sin^2\omega_0t}\right]$$

also

$$\left[\int_0^t \xi(t')dt'\right]^2 = \beta^2m^2\omega_0^4\left(\frac{x(t)-x(0)\cos\,\omega_0t}{\sin^2\omega_0t}\right)^2\left[\int_0^t \cos\,\omega_0(t-t')dt'\right]^2$$

$$= \beta^2m^2\omega_0^2\left(\frac{x^2(t)-2x(0)x(t)\cos\omega_0t+\,x^2(0)\cos^2\omega_0t}{\sin^2\omega_0t}\right)\,.$$

After R-differentiating (2.21) evaluating the result at $R = 0$, completing the square in $x(t)$ and $x(0)$, integrating and dividing the result by expression (2.18) gives the normalized

$$\frac{\partial}{\partial R} \langle G(x(t),x(0),\dot{x}(t),\dot{x}(0))\rangle \Big|_{R=0}$$

$$\begin{aligned} &= \frac{m^2\omega_0^2}{4} \{\frac{1}{m\beta}[(\frac{2\cos^2\omega_0 t}{\omega_0} - \frac{\cos\omega_0 t}{\omega_0})\frac{1}{m\beta} - (\frac{2\omega_0^3\cos\omega_0 t}{\sin\omega_0 t} \\ &+ \frac{\omega_0^3\cos^3\omega_0 t}{\sin\omega_0 t})\frac{1}{m^2\beta^2} + \frac{2\omega_0\cos^3\omega_0 t}{\sin^2\omega_0 t}] + \frac{1}{m^3\beta^3}[(\frac{-4\omega_0^2\cos^3\omega_0 t}{\sin^3\omega_0 t} \\ &- \frac{3\omega_0^2\cos\omega_0 t}{\sin^3\omega_0 t} + \frac{\omega_0^2\cos^5\omega_0 t}{\sin^3\omega_0 t} + \frac{4\omega_0^2\cos^2\omega_0 t}{\sin^3\omega_0 t} + \frac{20\omega_0^2\cos^5\omega_0 t}{\sin^3\omega_0 t} \\ &+ \frac{4\omega_0^4\cos^4\omega_0 t}{\sin^5\omega_0 t} - \frac{2\omega_0^4\cos^7\omega_0 t}{\sin^5\omega_0 t} - \frac{2\omega_0^4\cos^5\omega_0 t}{\sin^2\omega_0 t})]\} . \end{aligned} \tag{2.22}$$

To obtain $\langle S(0)S(t)\rangle$ requires taking the second time derivative of (2.22) but as this is of no immediate consequence it has not been done but only mentioned for completeness.

CHAPTER III

Imaginary Time Extension

It is known that an integral of an exponential always admits to a variational principle. However, in the present case the variational principle does not take the form of the more useful minimum principle. This is so because of the oscillatory nature of the complex exponential; therefore, if a useful principle is to be established the oscillation problem must be eliminated. This will be done by extending all the time factors to imaginary times, i.e. $t \to i\tau$ [18]. If transforms such as $\xi(i\tau) \to i\xi(\tau)$ are employed, then it is possible to guarantee a positive integrand, and consequently a rigorous bounding principle.

We will require $\int_0^\infty f(t)\,dt$ for even functions (i.e. $\frac{1}{2}\int_{-\infty}^{\infty} f(t)\,dt$). Assuming analyticity in the upper half complex time plane and sufficient fall off at infinity, we have the unique imaginary extension

$$f(i\tau) = \frac{1}{\pi}\int_{-\infty}^{\infty}\left(\frac{\tau}{t^2+\tau^2}\right) f(t)\,dt \; . \tag{3.1}$$

It follows that

$$\int_{-\infty}^{\infty} f(t)\,dt = \lim_{\tau\to\infty} \pi\tau f(i\tau) \; .$$

In practice, we will need extension to $\int_{-\infty}^{\infty} f(t)\, e^{i\omega t}\,dt$ (if only to allow $\omega \to 0+$ and therefore eliminate the constant component). Nevertheless the above considerations apply here as well:

$$(3.3) \qquad \int_{-\infty}^{\infty} f(t)\, e^{i\omega t}\, dt = \lim_{\tau\to\infty} \pi\tau f_\omega(i\tau)$$

where

$$(3.4) \qquad f_\omega(i\tau) = \frac{1}{\pi} \int_{-\infty}^{\infty} \left(\frac{\tau}{t^2+\tau^2}\right) e^{i\omega\tau}\, f(t)\, dt \ .$$

A concept somewhat similar to this is used in the Quantum statistical mechanical Green's function technique where the real Green's function at time = 0 is matched with its imaginary counterpart at time = $-i\beta$ (β is reciprocal temperature and $0 > \mathrm{Im}\,(t-t') > -\beta$). This essentially matches the real axis with a line through the imaginary axis, whereas we match the entire real line with a contour at infinity in the upper half plane.

A. Model of Time Extension.

As a demonstration of this idea (for $\omega \to 0+$) $f(t)$ is taken to be $J_0(t)$, the Bessel function of the first kind. Thus,

$$(3.5) \qquad \int_{-\infty}^{\infty} f(t)\, dt = \int_{-\infty}^{\infty} J_0(t)\, dt = 2$$

and it is known [24] that

$$(3.6) \qquad \frac{2}{\pi} \int_0^{\infty} \frac{\tau}{t^2+\tau^2}\, J_0(at)\, dt = [I_0(a\tau) - L_0(a\tau)]$$

with $a > 0$, $\mathrm{Re}\ \tau > 0$ and $I_0(a\tau) = \frac{1}{\pi}\int_0^{\pi} \cosh(a\tau \cos\theta)\, d\theta$ is the Bessel function of the second kind, while $L_0(a\tau) = \frac{2}{\pi} \int_0^{\pi/2} \sinh(a\tau \cos\theta)\, d\theta$ is the modified Sturve function. Thus,

$$(3.7)\quad \lim_{\tau\to\infty} \int_0^{\pi} \tau \cosh(\tau \cos \theta)d\theta - 2 \int_0^{\pi/2} \tau \sinh(\tau \cos \theta)\, d\theta$$

$$(3.8)\quad = \lim_{\tau\to\infty} 2 \int_0^{\pi/2} \tau\, e^{-\tau \cos \theta}\, d\theta$$

should give the same result as equation (3.5). But expression (3.8) can also be written as

$$(3.9)\quad \begin{aligned} &\lim_{\tau\to\infty} 2 \int_0^{\pi/2} \tau\, e^{-\tau \sin \theta}\, d\theta = \\ &\lim_{\tau\to\infty} 2 \int_0^{\infty} \tau\, e^{-\tau\theta}\, d\theta = 2\ ; \end{aligned}$$

and therefore the verification is made.

CHAPTER IV

Introduction.

We can now set up the required variational principle for transport coefficients, each of which can be written in the form $\int \lambda\, e^{-B} \ldots$ for $\lambda > 0$ and B real. This is done by observing that $\int \lambda(-B+1-\ln \rho)\rho = \int \lambda e^{-B}$ at $\rho = e^{-B}$, $\delta/\delta\rho \int \lambda(-B+1-\ln \rho)\rho = -\lambda(B+\ln \rho) = 0$ at $\rho = e^{-B}$ and $\delta^2/\delta\rho\,\delta\rho \int \lambda(-B+1-\ln \rho)\rho = -\lambda/\rho \leq 0$ for all $\rho \geq 0$. Hence setting $\rho = e^{-\bar{B}}$, we have the following lower bound inequality

$$(4.1) \qquad \int \lambda\, e^{-B} \ldots \geq \int \lambda(1+\bar{B}-B)\, e^{-\bar{B}} \ldots$$

(one obtains equality for $\bar{B}$ reducing to B). This enables one to make comparisons between a model system ($\bar{B}$) and another system (B) gaining information about the latter. As a simple test case this idea is applied to a model one-dimensional chain of oscillators and a second such system with different parameters. A simple exact inequality for the diffusion coefficient is obtained.

A. Decoupling the Hamiltonian [5,6]

We consider the Hamiltonian (neglecting end effects)

$$H = \sum_{j=1}^{N} (P_j^2/2m + cu_j^2) - \tfrac{1}{2} c \sum_{j=1}^{N} (u_j u_{j+1} + u_j u_{j-1})$$

$$= \sum_{j=1}^{N} (P_j^2/2m + cu_j^2) - c \sum_{j=1}^{N} u_j u_{j+1} \ .$$

The first term describes a set of independent harmonic oscillators, one on each site, while the second is the interaction between each oscillator and its nearest neighbor. By introducing the canonical transformation

$$(4.3) \qquad u_j = \frac{1}{\sqrt{N}} \sum_k \left(x_k \cos kjd - \frac{1}{m\omega_k} \Gamma_k \sin kjd\right)$$

$$(4.4) \qquad p_j = \frac{1}{\sqrt{N}} \sum_k \left(m\omega_k x_k \sin kjd + \Gamma_k \cos kjd\right)$$

where $\omega_k = \left[\frac{2c}{m} (1- \cos kd)\right]^{1/2}$

d = inter-oscillator distance

subject to the Poisson bracket rules

$$[x_k, \Gamma_k] = \delta_{kk'} \; , \qquad [x_k, x_{k'}] = [\Gamma_k, \Gamma_{k'}] = 0$$

we get after length manipulation

$$(4.5) \qquad H' = \sum_k \left(\frac{\Gamma_k^2}{2m} + \frac{m\omega_k^2}{2} x_k^2\right)$$

a completely decoupled[†] sum of ordinary harmonic oscillator Hamiltonians.

B. Simple Inequalities.

The diffusion coefficient can be written via $t \rightarrow i\tau$, in the form $\int \lambda \, e^{-B} \ldots$ and therefore the inequality holds and can be evaluated in any convenient form. With the intention of computing the diffusion coefficient equation (4.1) is made explicit by selecting

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[†] the usual transformation (see Chapter VI and Appendix A) leads to a Hamiltonain which mixes modes of wavenumber k and -k.

$$\lambda = e^{-\frac{1}{2}\sum_{k} R[\dot{x}_k(t)-\dot{x}_k(0)]^2}$$

$$\overline{B} = \sum_k [\tfrac{1}{2}\, m\beta\dot{x}_k^2(0)+ \tfrac{1}{2}\, A_k^{'}\beta x_k^2(0)- i\int_0^t \xi_k(t')(\dot{x}_k(t')$$

$$(4.6) \qquad - \dot{x}_k(0))dt' - \frac{i}{m}\int_0^t\int_0^{t'} \xi_k(t')A_k^{'}x_k(t'')dt'\, dt'']$$

$$B = \sum_k [\tfrac{1}{2}\, m\beta\dot{x}_k^2(0) + \tfrac{1}{2}\, A_k\beta x_k^2(0)- i\int_0^t \xi_k(t')(\dot{x}_k(t')$$

$$- \dot{x}_k(0))dt' - \frac{i}{m}\int_0^t\int_0^{t'} \xi_k(t')A_k x_k(t'')dt'\, dt''] \ ,$$

where $\Gamma_k(t) = m\dot{x}_k(t)$, $A_k = m\omega_k^2$, $A_k^{'} = m\overline{\omega}_k^2$.

As previously, we seek $<[\dot{x}_k(t)-\dot{x}_k(0)]^2> =$

$= - 2\,\frac{\partial}{\partial R} <e^{-\frac{1}{2}\sum_k R[\dot{x}_k(t)-\dot{x}_k(0)]^2}>\Big|_{R=0}$ so as to ultimately establish an inequality for the diffusion coefficient based upon its "model" value using $\overline{B}$. We will act as if normalization is automatic -- it is not in this case -- and show later how it can be made so.

Thus, the right hand side of (4.1) reduces to

$$(4.7) \qquad \int_{-\infty}^{\infty}\!\!\cdots\int_{-\infty}^{\infty} (1+ \sum_k [\tfrac{1}{2}(A_k-A_k^{'})\beta x_k^2(0)+ \frac{i}{m}\int_0^t\int_0^{t'} \xi_k(t')(A_k-A_k^{'})x_k(t'')$$

$$\cdot dt'dt'']) \exp \sum_k [- \tfrac{1}{2}\, R\dot{x}_k^2(t)+ R\dot{x}_k(t)\dot{x}_k(0)+ \tfrac{1}{2}\, R\dot{x}_k^2(0)$$

$$- \tfrac{1}{2}\, m\beta\dot{x}_k^2(0)- \tfrac{1}{2}\, A_k\ \ x_k^2(0)+ i\int_0^t \xi_k(t')(\dot{x}_k(t')-\dot{x}_k(0))\, dt' +$$

$$+ \frac{i}{m} \int_0^t \int_0^{t'} \xi_k(t')A_k x_k(t'')\, dt'\, dt'']$$

$$\cdot \prod_0^t d\xi(t') \prod_{0+}^{t-} dx_k(t')\, dx_k(0)\, dx_k(t)\, d\dot{x}_k(0) \ .$$

It should be observed that this kernel is apart from the summation over index k, essentially that dealt with in Chapter II and so by applying the same methods we can write for the kernel of (4.7)

$$(4.8) \quad \exp - \frac{1}{2} \sum_k (c_{11}x_k^2(0) + 2c_{12}x_k(0)x_k(t) + c_{22}x_k^2(t))$$

where the $x_k(t)$ are given by (2.9), the $\xi_k(t)$ by (2.10) and the c_{ij} are

$$c_{11} = \frac{\beta m\omega_0^2 + R\omega_0^2 \cos \omega_0 t + R}{R\omega_0^2 \cos \omega_0 t} \quad ; \quad c_{22} = \frac{\beta m\omega_0^2 + R\omega_0^2 \cos \omega_0 t - R}{\sin^2 \omega_0 t}$$

$$c_{12} = \frac{2\beta m\omega_0^2 \cos \omega_0 t}{\sin^2 \omega_0 t} + \frac{R\omega_0^2(1 + \cos^2 \omega_0 t)}{\sin^2 \omega_0 t} \ .$$

Hence, expression (4.7) after carrying through the lengthy but direct algebraic and differential operations is

$$(4.9) \quad \frac{\partial}{\partial R} \int \lambda(\overline{B} - B + 1)e^{-\overline{B}} \ldots \Big|_{R=0} = \sum_k \Big[\frac{1}{\beta m} \cos \omega_k t - \frac{1}{2\beta m}\Big(\frac{A_k}{m} - \frac{A_k'}{m}\Big) \sqrt{\frac{m}{A_k}} \Big(\frac{t \cos^2 \omega_k t}{\sin \omega_k t}\Big) \ ,$$

and for $A = A_k'$, one gets

$$(4.10) \quad \frac{\partial}{\partial R} \int \lambda\, e^{-\overline{B}} \ldots \Big|_{R=0} = \sum_k \frac{1}{\beta m} \cos \omega_k t \ .$$

Furthermore, the resultant contribution to the final inequality is

$$\frac{\partial}{\partial F} \int \lambda\, e^{-B} \ldots \Big|_{R=0} \leq \sum_k \Big[\frac{1}{\beta m} \cos \omega_k t - \frac{1}{2m\beta}\left(\frac{A_k}{m} - \frac{A_k'}{m}\right) \sqrt{\frac{m}{A_k}} \left(\frac{t \cos^2 \omega_k t}{\sin \omega_k t}\right)\Big] \tag{4.11}$$

where the sense of the inequality has changed because in taking the R-derivative a factor of -1 was brought across both sides of the equation. By combining these equations one establishes an inequality on the velocity autocorrelations between the model case and the second comparative system.

$$\begin{aligned} &<[\dot{x}_k(t)-\dot{x}_k(0)]^2> - <[\dot{x}_k(t)-\dot{x}_k(0)]^2>^M \\ &\leq \sum_k \frac{1}{2\beta\ A_k}\ \omega_k^2 (\bar{\omega}_k^2 - \omega_k^2) \left(\frac{t \cos^2 \omega_k t}{\omega_k \sin \omega_k t}\right) \end{aligned} \tag{4.12}$$

and perhaps a more convenient form of which is

$$\begin{aligned} &<[\dot{x}_k(t)-\dot{x}_k(0)]^2> - <[\dot{x}_k(t)-\dot{x}_k(0)]^2>^M \\ &\leq \sum_k \frac{1}{2\beta\ A_k} \left(\frac{A_k'}{A_k} - 1\right) \frac{\omega_k^3 t \cos^2 \omega_k t}{\sin \omega_k t} \end{aligned} \tag{4.13}$$

where $A_k' = A_k\ \bar{\omega}_k^2/\omega_k^2$.

C. Evaluation of Sums.

In order to evaluate this sum a transformation to an integral form will be made where for a system of N one-dimensional harmonic oscillators one has [19]

$$\frac{1}{N}\sum_k \cos\omega_k t \sim \frac{2}{\pi}\int_0^{\omega_L} \frac{\cos\omega t\, d\omega}{(\omega_L^2-\omega^2)^{1/2}}$$

for which the cutoff frequency is

$$m\omega_L^2 = 4A \quad \text{and} \quad g(\omega)\, d\omega = \frac{2\, d\omega}{\pi(\omega_L^2-\omega^2)^{1/2}}$$

is the fraction of circular frequencies between ω and $\omega + d\omega$, and

$$\frac{2}{\pi}\int_0^{\omega_L} \frac{\cos\omega t\, d\omega}{(\omega_L^2-\omega^2)^{1/2}} = J_0(\omega_L t) \quad \text{as} \quad N \to \infty\ .$$

Hence, returning to (4.10), we can write with the introduction of the cutoff frequency and spectral density

$$\begin{aligned} \frac{1}{N}\sum_k \frac{\omega_L^2}{4\beta A}\cos\omega_k t &\to - \frac{2}{\pi}\left(\frac{\omega_L^2}{4\beta A}\right)\int_0^{\omega_L} \frac{\cos\omega t}{(\omega_L^2-\omega^2)^{1/2}}\, d\omega \\ &= \frac{\omega_L^2}{4\beta A} J_0(\omega_L t)\ . \end{aligned} \tag{4.14}$$

Since the diffusion coefficient is readily obtained by integrating the (absolutely convergent) velocity-velocity correlation, we find

$$\begin{aligned} D &= \lim_{\underline{\omega}\to 0+}\int_0^\infty e^{i\underline{\omega} t} \langle \dot{x}(t)\dot{x}(0)\rangle\, dt \\ &= \int_0^\infty \frac{\omega_L^2}{4\beta A} J_0(\omega_L t)\, dt = \frac{\omega_L}{4\beta A} \end{aligned} \tag{4.15}$$

In like manner

$$
\begin{aligned}
&\frac{1}{N}\sum_k \frac{1}{2\beta\ A_k}\left(\frac{A_k'}{A_k}-1\right)\frac{t\omega_k^3\ \cos^2\omega_k t}{\sin\ \omega_k t} \\
(4.16)\quad & \\
&\rightarrow \frac{2}{\pi}\int_0^{\omega_L}\frac{1}{2\beta\ A_k}\left(\frac{A_k'}{A_k}-1\right)\frac{t\omega^3\ \cos^2\omega t\ d\omega}{(\sin\ \omega t)(\omega_L^2-\omega^2)^{1/2}}\ .
\end{aligned}
$$

For the sake of simplification in integration, we make the assumption that A_k and A_k' are independent of site and with the use of the trigonometric identity, $\cos^2\omega t + \sin^2\omega t = 1$, consider instead

$$
(4.17)\qquad \frac{1}{2\beta A}\left(\frac{A'}{A}-1\right)\int_0^{\omega_L}\frac{2t}{\pi}\ \frac{\omega^3}{(\omega_L^2-\omega^2)^{1/2}}\ \left(-\ \sin\ \omega t + \frac{1}{\sin\ \omega t}\right)d\omega.
$$

In order to establish the diffusion inequality, we break integral (4.17) into two parts and examine first

$$
(4.18)\lim_{a\to 0}\ \frac{1}{2\beta A}\left(\frac{A'}{A}-1\right)\int_0^{\infty}\int_0^{\omega_L}\frac{2}{\pi}\ \frac{\omega^3}{(\omega_L^2-\omega^2)^{1/2}}\ e^{-at}\ t\ \sin\ \omega t\ d\omega\ dt
$$

where e^{-at} is the usual convergence factor [*] and

$$
\lim_{a\to 0}\int_0^{\infty} e^{-at}\ t\ \sin\ \omega t\ dt = \frac{a}{a^2+\omega^2} \rightarrow 0
$$

thus (4.18) gives a zero contribution to the inequality. At this point let the imaginary time extension be made $t \rightarrow i\tau$ such that the second part of (4.17) becomes

$$
(4.19)\qquad \int_0^{\infty}\int_0^{\omega_L}\frac{\omega^3}{(\omega_L^2-\omega^2)^{1/2}}\ \frac{\tau}{\sinh\ \omega\tau}\ d\omega\ d\tau\ .
$$

---

[*] See J. L. Lebowitz and J. K. Percus, The Phys. Rev. 155, 1 (1967).

After carrying through the integration of (4.19) one gets

$$\frac{1}{2\beta A}\left(\frac{A'}{A}-1\right)\left(\frac{1}{2}\omega_L\right)$$

since the τ integral gives a factor of ω^{-2} and this, in turn, reduces the ω^3 integral to $\omega(\omega_L^2-\omega^2)^{-1/2}$ which yields ω_L. Thus, we have established

$$D - D^M \leq \frac{\omega_L}{4\beta A}\left(\frac{A'}{A}-1\right) \tag{4.20}$$

and (4.20) can be rewritten (see (4.15))

$$\frac{1}{A}-\frac{1}{A'} \leq \frac{1}{A}\left(\frac{A'}{A}-1\right)$$

which is equivalent to the second order error bound

$$(A'-A)^2 \geq 0 \ .$$

CHAPTER V

A direct comparison between an ordinary first order perturbation expansion for a quartic potential and a perturbation in the path integral formulation for the same potential will be made. The presence of certain oscillating terms in the path integral formulation will be eliminated by renormalizing about a frequency shifted harmonic term. In the full N-body problem a similar technique is employed.

A. The Ordinary Anharmonic Perturbation.

The one-body velocity auto-correlation generator expressed as a phase-space integral is

$$(5.1)\quad \langle e^{-\frac{1}{2}R\dot{x}(t)\dot{x}(0)}\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{1}{2}R\dot{x}(t)\dot{x}(0)} \cdot e^{-\beta H(x(0),\dot{x}(0))}\, dx(0)\, d\dot{x}(0) \quad ;$$

in this equation the hamiltonian is

$$H(x(t),\dot{x}(t)) = H_0 + H_1$$

where

$$H_0 = \frac{1}{2}m\dot{x}^2(t) + \frac{1}{2}m\omega_0^2x^2(t) \quad \text{and} \quad H_1 = -\frac{1}{2}\left(\frac{m\omega_0^2\mu}{12}\right)x^4(t) \ .$$

The corresponding equation of motion is

$$(5.2)\qquad m\ddot{x}(\tau) + m\omega_0^2x(\tau) - \frac{m\omega_0^2\mu}{6}x^3(\tau) = 0$$

with solution [25], to first order in μ, given by

$x(\tau) = x_0(\tau) + \mu x_1(\tau)$, where

$$(5.3)\quad x_0(\tau) = (x_0(t)\sin \omega_0\tau + x_0(0)\sin \omega_0(t-\tau))/\sin \omega_0 t$$

and

$$(5.4)\quad x_1(\tau) = \frac{1}{192}\left[x_0^3(0) - 3x_0(0)\left(\frac{x_0(t)-x_0(0)\cos \omega_0 t}{\sin \omega_0 t}\right)^2\right]$$

$$\cdot[\cos 3\omega_0\tau - \cos \omega_0\tau] + \frac{3}{192}\left[\left(\frac{x_0(t)-x_0(0)\cos \omega_0 t}{\sin \omega_0 t}\right)^3\right.$$

$$\left. -3x_0^2(0)\left(\frac{x_0(t)-x_0(0)\cos \omega_0 t}{\sin \omega_0 t}\right)\right]\left[\frac{1}{3}\sin 3\omega_0\tau - \sin \omega_0\tau\right]$$

subject to the conditions

$$\dot{x}(0) = \dot{x}_0(0)\ ; \qquad \dot{x}_1(0) = 0$$

$$x(0) = x_0(0)\ ; \qquad x_1(0) = 0\ .$$

Therefore (5.1) becomes after expanding to first order in μ

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{1}{2}R\dot{x}_0(t)\dot{x}_0(0)}\, e^{-\frac{1}{2}m\beta\dot{x}_0^2(0)}$$

$$(5.5)\quad \cdot e^{-\frac{1}{2}m\beta\omega_0^2x_0^2(0)}\left(1+\frac{\mu m\beta\omega_0^2x_0^4(0)}{24} - \frac{\mu R\dot{x}_1(t)\dot{x}_0(0)}{2} + \ldots\right)D[\ldots]$$

$$= \frac{2\pi}{\sqrt{\alpha\theta}}\left(1+\frac{\mu m\beta\omega_0^2}{24\theta^2} + \left[\frac{3\mu R}{384}\omega_0\sin 3\omega_0 t + \frac{\mu R}{384}\omega_0\sin \omega_0 t\right]\right.$$

$$\left.\cdot\left[\frac{R\omega_0\sin \omega_0 t}{2\alpha\theta^2} - \frac{9R\sin \omega_0 t}{2\omega_0\alpha^2\theta} - \frac{3R^3\omega_0\sin^3\omega_0 t}{8\alpha^3\theta^3}\right]\right)\ ,$$

where $\alpha = R\cos \omega_0 t + m\beta$

$$\theta = \omega_0\left[m\beta - \frac{R^2\sin^2\omega_0 t}{4(R\cos \omega_0 t + m\beta)}\right]$$

B. Path Integral Perturbation.

We now ask that this integral give the same result[†] as the path expression

$$\langle e^{-\frac{1}{2}R\dot{x}(t)\dot{x}(0)}\rangle = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} e^{-\frac{1}{2}R\dot{x}(t)\dot{x}(0)}\, e^{-\frac{1}{2}m\beta\dot{x}^{2}(0)}$$

$$\text{(5.6)}\quad \cdot\, e^{-\frac{1}{2}m\beta(\omega_0^2x^2(0)-\frac{\omega_0^2\mu x^4(0)}{12})}\,\exp[i\int_0^t \xi(t')(\dot{x}(t')-\dot{x}(0))dt'$$

$$+\, i\int_0^t\int_0^{t'}(\omega_0^2-\Omega^2)\xi(t')x(t'')\,dt'\,dt'' - \frac{i}{m}\int_0^t\int_0^{t'}\xi(t')F(x(t''))dt'dt'']$$

$$\cdot \prod_0^t d\xi(t') \prod_{0+}^{t-} dx(t')\,dx(0)\,dx(t)\,d\dot{x}(0)\ ,$$

where Ω^2 represents the frequency shift term about which renormalization will be performed and $F(x(t''))$ contains the cubic force and linear force terms. Simultaneously putting the kernel into the quadratic square form and expanding one obtains[††]

$$\text{(5.7)}\quad \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \exp -\frac{1}{2m\beta}[\int_0^t\int_0^{t'} \xi(t')\xi(t'')\,dt'\,dt''-iR\dot{x}(t)\int_0^t\xi(t')dt'$$

$$-\,\frac{1}{4}R^2\dot{x}^2(t)]e^{-\frac{1}{2}m\beta\omega_0^2x^2(0)}\ e^{i\int_0^t \xi(t')\dot{x}(t')dt'}$$

$$\cdot\, e^{i\omega_0^2\int_0^t\int_0^{t'}\xi(t')x(t'')dt'dt''}\ e^{-i\Omega^2\int_0^t\int_0^{t'}\xi(t')x(t'')dt'dt''}$$

$$\cdot(1+\frac{\mu m\beta\omega_0^2x^4(0)}{24} - i\int_0^t\int_0^{t'}\frac{\omega_0^2\mu}{6}\xi(t')x^3(t'')dt'dt''+$$

[†] to within a Jacobian transformation factor between coordinate sets $(\dot{x}(0),x(0))$ and $(x(t),x(0))$ which is essentially the normalization discussed in Chapter II and, since we are going to renormalize, is not included.

[††] See Appendix E for integration of linear terms in the functional integral and Chapter VI Section C for further discussion of the frequency shift.

$$+ i \int_0^t \int_0^{t'} \Omega^2 \xi(t')x(t'')\, dt'\, dt'')\, D[\ldots]\ .$$

C. Comparison of the Integral Forms.

We will now compare the exponents of (5.1) and (5.7) without the frequency shift, although the shift is of course required to annul the secular terms in general. Certainly upon $x(0)$, $\dot{x}(0)$ integration, the exponents come down to the integrand, and hence will occur together with the explicit integrand of the above. The required integrations are not easy. However, our major interest is in long time dependence. We shall show that in this limit, explicit integrands become identical without frequency shift. Hence exponents are identical too, and further integrations are not necessary to establish identity of the two methods. With this in mind expression (5.7) can be written

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{1}{2}(c_{11}x^2(0)+2c_{12}x(0)x(t)+c_{22}x^2(t))}$$

$$(5.8)\qquad \cdot\Big(1 + \frac{\mu m\beta\omega_0^2 x^4(0)}{24} - i\int_0^t\int_0^{t'} \frac{\omega_0^2\mu}{6}\, \xi_s(t')x_s^3(t'')dt'dt''$$

$$+i\int_0^t\int_0^{t'} \Omega^2\ \xi_s(t')x_s(t'')\ dt'\ dt''\Big)\ dx(0)\ dx(t)\ ,$$

where $\xi_s(t')$, $x_s(t'')$ are $\xi(t')$, $x(t'')$ evaluated at the saddle point and are given by (2.9), (2.10) and the c_{ij} are given by (2.14).

The solution of equation (5.2) has been so constructed that its zero-th order portion is exactly that obtained by solving the variational equations of the path integral for the one-body oscillator[†]. An immediate observation is that the zero subscript can be placed on all x or $\dot{x}$. Thus directly comparing the kernels

$$\begin{aligned}
&\exp -\tfrac{1}{2}(c_{11}x_0^2(0)+ 2c_{12}x_0(0)x_0(t)+ c_{22}x_0^2(t)) \\
&= \exp -\tfrac{1}{2}\,[\{(\beta m\omega_0^2+ R\omega_0^2 \cos \omega_0 t)/\sin^2\omega_0 t\} \\
&\quad\cdot(x_0^2(0)+ x_0^2(0) \cos^2 \omega_0 t + \dot{x}_0^2(0) \sin^2 \omega_0 t/\omega_0^2 \\
&\quad + 2\dot{x}_0(0)x_0(0) \cos \omega_0 t \sin \omega_0 t /\omega_0) - 2\{(\tfrac{1}{2} R\omega_0^2 \\
&\quad + \tfrac{1}{2} R\omega_0^2 \cos^2\omega_0 t + \beta m\omega_0^2 \cos \omega_0 t)/\sin^2\omega_0 t\} \\
&\quad\cdot(x_0^2(0) \cos \omega_0 t + x_0(0)\dot{x}_0(0) \sin \omega_0 t /\omega_0)]
\end{aligned} \tag{5.9}$$

since

$$\dot{x}_0(\tau)\Big|_{\tau=0} \text{ gives } x_0(t) = x_0(0)\cos \omega_0 t + \dot{x}_0(0)\sin \omega_0 t/\omega_0. \tag{5.10}$$

After further algebra, this can be reduced to

$$\begin{aligned}
&\exp -\tfrac{1}{2} R\omega_0^2[\dot{x}_0(0)x_0(0) \cos^2\omega_0 t \,/\, \omega_0 \sin \omega_0 t \\
&\quad + \dot{x}_0^2(0) \cos \omega_0 t/\omega_0 - \dot{x}_0(0)x_0(0)/\omega_0 \sin \omega_0 t] \\
&\quad\cdot e^{-\frac{1}{2} m\beta\dot{x}_0^2(0)}\, e^{-\frac{1}{2} m\beta\omega_0^2x_0^2(0)} ,
\end{aligned}$$

[†] see conditions (5.4).

which in fact corresponds to

$$(5.11)\quad \exp - \tfrac{1}{2} R\, \dot{x}_0(t)\dot{x}_0(0)\; e^{-\frac{1}{2}m\beta\dot{x}_0^2(0)}\; e^{-\frac{1}{2}m\beta\omega_0^2 x_0^2(0)}$$

since $\dot{x}_0(\tau)\Big|_{\tau=t}$ gives

$$(5.12)\qquad \frac{\dot{x}_0(t)}{\omega_0} = \frac{x_0(t)\cos\omega_0 t - x_0(0)}{\sin\omega_0 t}$$

and $x_0(t)$ is given by (5.10).

It remains now to directly compare the integrands; thus

$$-\mu R\dot{x}_1(t)\dot{x}_0(0) = -\mu R\{\frac{1}{192}[x_0^3(0)\dot{x}_0(0) - \frac{3x_0(0)\dot{x}_0^3(0)}{\omega_0^2}]$$

$$(5.13)\cdot[-3\omega_0 \sin 3\omega_0 t + \omega_0 \sin\omega_0 t] + \frac{3}{192}[\frac{\dot{x}_0^4(0)}{\omega_0^3} - 3x_0^2(0)\dot{x}_0^2(0)/\omega_0]$$

$$\cdot[\omega_0\cos 3\omega_0 t - \omega_0 \cos\omega_0 t]\}$$

should give the same result as

$$(5.14)\quad -\,i\int_0^t\int_0^{t'} \frac{\omega_0^2\mu}{6}\,\xi(t')x^3(t'')\,dt'\,dt''$$

after various terms are renormalized. Here $\xi(t')$ and $x(t'')$ have the same form as (2.9) and (2.10) so that when this integral is expanded out one has only to evaluate the following four terms.

$$\int_0^t\int_0^{t'} \cos\omega_0\,(t-t')\,\sin^3\omega_0 t''\,dt'\,dt''$$

$$= -\frac{1}{3\omega_0}[-\frac{\cos\omega_0 t\,\sin 4\omega_0 t}{32\omega_0} + \frac{\sin\omega_0 t}{4}(\frac{1}{2\omega_0} - \frac{\cos 2\omega_0 t}{2\omega_0})$$

$$-\frac{\sin\omega_0 t}{8}(\frac{1}{4\omega_0} - \frac{\cos 4\omega_0 t}{4\omega_0})] - \frac{2}{3\omega_0}[\frac{\cos\omega_0 t\,\sin 2\omega_0 t}{4\omega_0} + \frac{\sin\omega_0 t}{4\omega_0} -$$

$$-\frac{\sin\omega_0 t\cos 2\omega_0 t}{4\omega_0}] + \frac{2\sin\omega_0 t}{3\omega_0^2}$$

$$\int_0^t\int_0^{t'} \cos\omega_0(t-t')\sin^3\omega_0(t-t'')\,dt'\,dt'' =$$

$$-\frac{1}{96\omega_0^2}\sin 4\omega_0 t - \frac{1}{6\omega_0^2}\sin 2\omega_0 t - \frac{1}{9\omega_0^2}[3\sin^3\omega_0 t\cos\omega_0 t$$

$$-6\cos\omega_0 t\sin\omega_0 t]$$

$$\int_0^t\int_0^{t'} \cos\omega_0(t-t')\sin^2\omega_0 t''\sin\omega_0(t-t'')\,dt'\,dt'' =$$

$$\frac{\sin\omega_0 t}{3\omega_0}[\cos\omega_0 t(\frac{1}{4\omega_0} - \frac{\cos 2\omega_0 t}{4\omega_0}) - \frac{\sin\omega_0 t\sin 2\omega_0 t}{4\omega_0}$$

$$-\cos\omega_0 t(\frac{1}{8\omega_0} - \frac{\cos 2\omega_0 t}{8\omega_0}) - \cos\omega_0 t(\frac{1}{32\omega_0} - \frac{\cos 4\omega_0 t}{32\omega_0})$$

$$+\frac{\sin\omega_0 t\sin 4\omega_0 t}{32\omega_0}] + \frac{\cos\omega_0 t}{3\omega_0}[-\frac{\cos\omega_0 t\sin 4\omega_0 t}{32\omega_0}$$

$$+\sin\omega_0 t(\frac{1}{8\omega_0} - \frac{\cos 2\omega_0 t}{8\omega_0}) - \sin\omega_0 t(\frac{1}{32\omega_0} - \frac{\cos 4\omega_0 t}{32\omega_0})] + \frac{2\cos\omega_0 t}{3\omega_0}$$

$$[\frac{\cos\omega_0 t\sin 2\omega_0 t}{4\omega_0} + \sin\omega_0 t(\frac{1}{4\omega_0} - \frac{\cos 2\omega_0 t}{4\omega_0})] - \frac{2\cos\omega_0 t\sin\omega_0 t}{3\omega_0^2}$$

$$\int_0^t\int_0^{t'} \cos\omega_0(t-t')\sin\omega_0 t''\sin^2\omega_0(t-t'')\,dt'\,dt''$$

$$= -\frac{\sin\omega_0 t}{3\omega_0}[\frac{\sin 4\omega_0 t}{32\omega_0} + (\frac{\cos 2\omega_0 t}{4\omega_0} - \frac{1}{4\omega_0})] - \frac{\cos\omega_0 t}{3\omega_0}[-\frac{\sin 4\omega_0 t}{32\omega_0}$$

$$-\frac{\sin 2\omega_0 t}{2\omega_0}] + \frac{\sin\omega_0 t}{\omega_0}[+\frac{\sin^2\omega_0 t + 2\cos^2\omega_0 t}{3\omega_0}]$$

Therefore equation (5.14) after algebraic manipulation is

$$[\frac{\mu\beta m\omega_0^3\dot{x}_0(0)}{6} + \frac{\mu R\omega_0^4}{12}(\frac{\dot{x}_0(0)}{\omega_0}\cos\omega_0 t - x_0(0)\sin\omega_0 t)]$$

$$\cdot\{(\frac{\dot{x}_0^3(0)}{\omega_0^3} + \frac{3\dot{x}_0^2(0)x_0(0)\cos\omega_0 t}{\omega_0^2\sin\omega_0 t} + \frac{3\dot{x}_0(0)x_0^2(0)\cos^2\omega_0 t}{\omega_0\sin^2\omega_0 t}$$

$$+ \frac{x_0^3(0)\cos^3\omega_0 t}{\sin^3\omega_0 t})(-\frac{1}{3\omega_0}[-\frac{\cos\omega_0 t\sin 4\omega_0 t}{32\omega_0} + \frac{\sin\omega_0 t}{8\omega_0}$$

$$-\frac{\sin\omega_0 t\cos 2\omega_0 t}{8\omega_0} - \frac{\sin\omega_0 t}{32\omega_0} + \frac{\sin\omega_0 t\cos 4\omega_0 t}{32\omega_0}] -$$

$$-\frac{2}{3\omega_0}[\frac{\cos\omega_0 t\sin 2\omega_0 t}{4\omega_0} - \frac{\sin\omega_0 t\cos 2\omega_0 t}{4\omega_0} + \frac{\sin\omega_0 t}{4\omega_0} - \frac{\sin\omega_0 t}{\omega_0}])$$

$$+ 3(\frac{\dot{x}_0(0)x_0^2(0)}{\omega_0\sin^2\omega_0 t} + \frac{x_0^3(0)\cos\omega_0 t}{\sin^3\omega_0 t})(-\frac{\sin\omega_0 t}{3\omega_0}[\frac{\sin 4\omega_0 t}{32\omega_0} + \frac{\cos 2\omega_0 t}{4\omega_0}$$

$$-\frac{1}{4\omega_0}] - \frac{\cos\omega_0 t}{3\omega_0}[-\frac{\sin 4\omega_0 t}{32\omega_0} - \frac{\sin 2\omega_0 t}{2\omega_0}] - \frac{\sin\omega_0 t}{\omega_0}[-\frac{\sin^2\omega_0 t}{3\omega_0}$$

$$-\frac{2\cos^2\omega_0 t}{3\omega_0}]) + 3(\frac{\dot{x}_0^2(0)x_0(0)}{\omega_0^2\sin\omega_0 t} + \frac{2\dot{x}_0(0)x_0^2(0)\cos\omega_0 t}{\omega_0\sin^2\omega_0 t} + \frac{x_0^3(0)\cos^2\omega_0 t}{\sin^3\omega_0 t})$$

$$\cdot(\frac{\sin\omega_0 t\cos\omega_0 t}{3\omega_0}[\frac{}{4\omega_0} - \frac{\cos\omega_0 t\cos 2\omega_0 t}{4\omega_0} - \frac{\sin\omega_0 t\sin 2\omega_0 t}{4\omega_0} - \frac{\cos\omega_0 t}{8\omega_0}$$

$$+ \frac{\cos\omega_0 t\cos 2\omega_0 t}{8\omega_0} - \frac{\cos\omega_0 t}{32\omega_0} + \frac{\cos\omega_0 t\cos 4\omega_0 t}{32\omega_0} + \frac{\sin\omega_0 t\sin 4\omega_0 t}{32\omega_0}]$$

$$+ \frac{\cos\omega_0 t}{3\omega_0}[-\frac{\cos\omega_0 t\sin 4\omega_0 t}{32\omega_0} + \frac{\sin\omega_0 t}{8\omega_0} - \frac{\sin\omega_0 t\cos 2\omega_0 t}{8\omega_0}$$

$$-\frac{\sin\omega_0 t}{32\omega_0} + \frac{\sin\omega_0 t\cos 4\omega_0 t}{32\omega_0} + \frac{\cos\omega_0 t\sin 2\omega_0 t}{2\omega_0} + \frac{\sin\omega_0 t}{2\omega_0}$$

$$-\frac{\sin\omega_0 t\cos 2\omega_0 t}{2\omega_0} - \frac{2\sin\omega_0 t}{\omega_0}]) + \frac{x_0^3(0)}{\sin^3\omega_0 t}(-\frac{1}{96\omega_0}\sin 4\omega_0 t$$

$$-\frac{\sin 2\omega_0 t}{6\omega_0^2} - \frac{\sin^3\omega_0 t\cos\omega_0 t}{3\omega_0^2} + \frac{2\cos\omega_0 t\sin\omega_0 t}{3\omega_0^2})\}$$

D. Renormalization of Terms

We now search expression (5.14) for typical terms which correspond to those of (5.13). The first such term is

$$(5.15)\quad -\left(\frac{3x_0(0)\dot{x}_0^3(0)}{192\omega_0}\right)(3\sin 3\omega_0 t - \sin\omega_0 t)\ ;$$

a corresponding term arising from (5.14) is

$$-\frac{1}{6(192)}\,\frac{x_0(0)\dot{x}_0^3(0)}{\omega_0}\cos\omega_0 t\sin 4\omega_0 t$$

$$= \frac{1}{3(192)}\,\frac{x_0(0)\dot{x}_0^3(0)}{\omega_0}\left\{\frac{3}{4}\sin 3\omega_0 t - \frac{1}{4}\sin\omega_0 t - \sin^2\omega_0 t\sin 3\omega_0 t\right\}$$

since

$$\cos\omega_0 t\sin\omega_0 t = 2(1-\sin^2\omega_0 t)(\sin 3\omega_0 t - \sin\omega_0 t)$$

$$\sin^3\omega_0 t = -\frac{1}{4}\sin 3\omega_0 t + \frac{3}{4}\sin\omega_0 t\ .$$

Therefore the terms will have the same structure provided that

$$\frac{1}{3(192)}\,\frac{1}{\omega_0}\,x_0(0)\dot{x}_0^3(0)\sin^2\omega_0 t\sin 3\omega_0 t$$

can be balanced by the secular term coming from the frequency shifted harmonic contribution. Another contributor to (5.15) is

$$\frac{1}{2(192)}\,\frac{x_0(0)\dot{x}_0^3(0)}{\omega_0}\cos\omega_0 t\sin 4\omega_0 t$$

which can be converted to

$$\frac{1}{(3)(4)(192)}\,\frac{1}{\omega_0}\,x_0(0)\dot{x}_0^3(0)\left\{\sin 3\omega_0 t - \frac{1}{3}\sin\omega_0 t\right\}$$

leaving also a portion to be balanced off. Furthermore, other such terms exist and can be handled in like manner.

A second distinct typical term is

$$(5.16) \qquad - \frac{3}{192} \frac{\dot{x}_0^4(0)}{\omega_0^2} (\cos 3\omega_0 t - \cos \omega_0 t)$$

a correspondence comes from

$$- \frac{1}{6(192)} \frac{1}{\omega_0^2} \dot{x}_0^4(0) \frac{\cos \omega_0 t}{\sin \omega_0 t} (\sin \omega_0 t \cos 4\omega_0 t)$$

and since

$$\cos \omega_0 t \cos 4\omega_0 t = \frac{3}{2}(\cos 3\omega_0 t - \cos \omega_0 t)$$
$$+ (\cos \omega_0 t - 2 \sin^2 \omega_0 t \cos 3\omega_0 t),$$

we obtain

$$- \frac{1}{4(192)} \frac{\dot{x}_0^4(0)}{\omega_0^2} (\cos 3\omega_0 t - \cos \omega_0 t)$$

plus a portion to be renormalized. The remaining two characteristic terms are

$$(5.17) \quad - \frac{1}{192} x_0^3(0)\dot{x}_0(0)(-3\omega_0 \sin 3\omega_0 t + \omega_0 \sin \omega_0 t)$$

and

$$(5.18) \quad - \frac{9}{192} x_0^2(0)\dot{x}_0^2(0)(\cos 3\omega_0 t - \cos \omega_0 t) ,$$

and their corresponding components are treatable in analogous fashion. Thus, we see by judiciously balancing terms we can get the integrands to be identical.

It is to be recalled that we are interested in

$$<\dot{x}(t)\dot{x}(0)> = - 2 \frac{\partial}{\partial R} <e^{- \frac{1}{2} R\dot{x}(t)\dot{x}(0)}>\Big|_{R=0}$$

and hence can discard all R terms in the examination of the shifted frequency term viz. its R dependence being superfluous following the differentiation procedure. Whereupon after the frequency shift term of (5.8) is integrated and all remaining renormalizable terms are collected simple algebra gives:

$$(5.19)\quad \Omega^2 = \mu\omega_0^2\dot{x}_0(0)\{(\frac{\dot{x}_0^3(0)}{\omega_0^3}\sin^3\omega_0 t + \frac{3\dot{x}_0^2(0)x_0(0)}{\omega_0^2}\cos\omega_0 t\sin^2\omega_0 t$$

$$+\frac{3\dot{x}_0(0)x_0^2(0)\cos^2\omega_0 t\sin\omega_0 t}{\omega_0} + x_0^3(0)\cos^3\omega_0 t)(-\frac{1}{3\omega_0}$$

$$\cdot[-\frac{\cos\omega_0 t\sin 4\omega_0 t}{32\omega_0} + \frac{3\sin\omega_0 t}{32\omega_0} - \frac{\sin\omega_0 t\cos 2\omega_0 t}{8\omega_0}$$

$$+\frac{\sin\omega_0 t\cos 4\omega_0 t}{32\omega_0} - \frac{\cos\omega_0 t\sin 2\omega_0 t}{2\omega_0} - \frac{\sin\omega_0 t\cos\omega_0 t}{2\omega_0}$$

$$-\frac{3\sin\omega_0 t}{2\omega_0}]) + 3(\frac{\dot{x}_0(0)x_0^2(0)}{\omega_0}\sin\omega_0 t + x_0^3(0)\cos\omega_0 t)(-\frac{\sin\omega_0 t}{3\omega_0}$$

$$\cdot[\frac{\sin 4\omega_0 t}{32\omega_0} + \frac{\cos 2\omega_0 t}{4\omega_0} - \frac{1}{4\omega_0}] - \frac{\cos\omega_0 t}{3\omega_0}[-\frac{\sin 4\omega_0 t}{32\omega_0} - \frac{\sin 2\omega_0 t}{2\omega_0}]$$

$$-\frac{\sin\omega_0 t}{\omega_0}[-\frac{\sin^2\omega_0 t}{3\omega_0} - \frac{2\cos^2\omega_0 t}{3\omega_0}]) + 3(\frac{\dot{x}_0^2(0)x_0(0)}{\omega_0^2}\sin^2\omega_0 t$$

$$+\frac{2\dot{x}_0(0)x_0^2(0)\cos\omega_0 t\sin\omega_0 t}{\omega_0^2} + x_0^3(0)\cos^2\omega_0 t)(\frac{\sin\omega_0 t}{3\omega_0}[\frac{\cos\omega_0 t}{4\omega_0}$$

$$-\frac{\cos\omega_0 t\cos 2\omega_0 t}{4\omega_0} - \frac{\sin\omega_0 t\sin 2\omega_0 t}{4\omega_0} - \frac{\cos\omega_0 t}{8\omega_0}$$

$$+\frac{\cos\omega_0 t\cos 2\omega_0 t}{8\omega_0} - \frac{\cos\omega_0 t}{32\omega_0} + \frac{\cos\omega_0 t\cos 4\omega_0 t}{32\omega_0} + \frac{\sin\omega_0 t\sin 4\omega_0 t}{32\omega_0}]$$

$$+\frac{\cos\omega_0 t}{3\omega_0}[-\frac{\cos\omega_0 t\sin 4\omega_0 t}{32\omega_0} + \frac{\sin\omega_0 t}{8\omega_0} - \frac{\sin\omega_0 t\cos 2\omega_0 t}{8\omega_0} -$$

$$- \frac{\sin \omega_0 t}{32\omega_0} + \frac{\sin \omega_0 t \cos 4\omega_0 t}{32\omega_0} + \frac{\cos \omega_0 t \sin 2\omega_0 t}{2\omega_0} + \frac{\sin \omega_0 t}{2\omega_0}$$

$$- \frac{\sin \omega_0 t \cos 2\omega_0 t}{2\omega_0} - \frac{2 \sin \omega_0 t}{\omega_0}]) + \dot{x}_0^3(0)(- \frac{\sin 4\omega_0 t}{96\omega_0}$$

$$- \frac{\sin 2\omega_0 t}{6\omega_0^2} - \frac{\sin^3 \omega_0 t \cos \omega_0 t}{3\omega_0^2} + \frac{2 \cos \omega_0 t \sin \omega_0 t}{3\omega_0^2})\}$$

$$/\{(x_0^2(t) - x_0(0)x_0(t) \cos \omega_0 t)(\frac{\sin \omega_0 t}{2\omega_0} - \frac{t \cos \omega_0 t}{2})$$

$$+ (x_0(0)x_0(t) - x_0^2(0) \cos \omega_0 t)(\frac{t}{2} - \frac{t \cos \omega_0 t}{2} + \frac{\sin 2\omega_0 t}{4\omega_0} - \frac{\sin \omega_0 t}{2\omega_0})\}$$

Now as $t \to \infty$ the numerator has oscillating sine and cosine terms whereas in the denominator the secular t term goes to infinity indicating that $\Omega^2 \to 0$ in the long time limit.[†] We explicitly write

$$(x_0^2(t) - x_0(0)x_0(t) \cos \omega_0 t)(- \tfrac{1}{2}\, t \cos \omega_0 t) + (x_0(0)x_0(t)$$

$$- x_0^2(0) \cos \omega_0 t)(\tfrac{1}{2}\, t)(1 - \cos \omega_0 t)$$

$$= [x_0(0)\dot{x}_0(0)(\sin \omega_0 t - \sin \omega_0 t \cos \omega_0 t) - x_0(0)\dot{x}_0(0) \sin \omega_0 t \cos^2 \omega_0 t$$

$$- \dot{x}_0^2(0) \sin^2 \omega_0 t \cos \omega_0 t / \omega_0] \frac{t}{2\omega_0} ,$$

since $x_0(t) = x_0(0) \cos \omega_0 t + \dot{x}_0(0) \sin \omega_0 t / \omega_0$.

The coefficient of the t term is

$$\dot{x}_0(0) \sin \omega_0 t [x_0(0)(1 - \cos \omega_0 t) - x_0(0) \cos^2 \omega_0 t - \dot{x}_0(0) \sin \omega_0 t \cos \omega_0 t / \omega_0] , \qquad (5.20)$$

[†] this can be seen to be true for the imaginary time case as well viz. see Appendix D.III.

and the sin $\omega_0 t$ factor can be cancelled since each term in the numerator has a like factor. Therefore, we must now check the coefficient to make sure that it does not go through zero.

E. Examination of Secular Coefficient.

If the coefficient did become zero for some values of $\dot{x}_0(0)$ and $x_0(0)$ we would have

$$(5.21)\quad x_0(0)(1-\cos\omega_0 t-\cos^2\omega_0 t)-\frac{\dot{x}_0(0)}{\omega_0}\cos\omega_0 t\sqrt{1-\cos^2\omega_0 t}=0;$$

transposing, squaring and collecting like terms gives

$$(5.22)\quad c^4+2q\,c^3-c^2-2q\,c+q=0$$

where $c=\cos\omega_0 t$ and $q=x_0^2(0)/(x_0^2(0)+\dot{x}_0^2(0)/\omega_0^2)$.

Upon examining[†] equation (5.22) one finds that the roots of the quartic are complex and hence the coefficient of the t term cannot reach zero for any real values of $\cos\omega_0 t$. Thus the two perturbation forms give the same result.

[†] See Appendix F.

The path integral representation is now called upon to handle the N-body problem of transport in a Debye-type crystal with nearest neighbor cubic forces. To guarantee normalization, start with a system for which an exact solution is known and turn on the remaining potential from $-\infty < t \leq 0$ as $\lim_{\gamma\to 0} \Phi(t) = \Phi_H + \Phi_Q\, e^{\gamma t}$ (where e.g. Φ_H = harmonic and Φ_Q = quartic). The density subject to $\partial\rho/\partial t + v\cdot\partial\rho/\partial x + \dot{v}\cdot\partial\rho/\partial v = 0$ will have its normalization maintained since $\partial/\partial t \int \rho\, dx\, dv = 0$ and the initial entropy is unchanged. Then at time = t one inquires as to the correlation of the one-body phase-space density with that at time = 0, allowing the calculation of transport coefficients.

In particular, we will determine an inequality for the velocity-velocity correlation function in the infinite imaginary time limit. For nearest neighbor type forces

$$(6.1)\quad f_s(x(t'')) = -\sum_j \tilde{A}_{sj}(x_s-x_j)^3 + \sum_j m\,\tilde{\Omega}^2_{sj}(x_s-x_j)$$

where $x_i = x_i(t'')$; $s = j \pm 1$ and the corresponding Hamiltonian is

$$(6.2)\quad H = \sum_s \frac{P_s^2}{2m} + \sum_{s,j} \frac{1}{4}\tilde{A}_{sj}(x_s-x_j)^4 - \sum_{s,j} \frac{1}{2} m\tilde{\Omega}^2_{sj}(x_s-x_j)^2 .$$

A. Normal Mode Transformations[†]

To transform to normal mode variables one writes the deviation from particle position as

$$(6.3) \qquad x_j(t) = \sum_k \frac{1}{\sqrt{M}} \exp \frac{2\pi ijk}{M} \, x(k,t) + j$$

and time differentiating gives

$$(6.4) \qquad \dot{x}_j(t) = \sum_k \frac{1}{\sqrt{M}} \exp \frac{2\pi ijk}{M} \, \dot{x}(k,t) \ .$$

Likewise the conjugate variable is expressed as

$$(6.5) \qquad \xi_j(t) = \sum_k \frac{1}{\sqrt{M}} \exp \frac{2\pi ijk}{M} \quad (k,t)$$

with lattice modes j = 1,2,...,M and k = 1,2,...,M.

To apply these transformations use will be made of

$$(6.6) \qquad \sum_j \frac{1}{\sqrt{M}} e^{2\pi ijk/M} \frac{1}{\sqrt{M}} e^{-2\pi ij\ell/M} = \delta_{k\ell}$$

and

$$(6.7) \qquad \sum_{k,\ell} \frac{A_{k\ell}}{M} e^{2\pi in\ell/M} e^{-2\pi ink/M} = m\omega_n^2 \ .$$

We will again want the integral from $t = 0$ to $t = i\infty$

$$\lim_{\underline{\omega}\to 0+} \left[\int \lambda \, e^{-B} \ldots \geq \int \lambda(-B+1-\ln \rho)\rho \ldots = \int \lambda(\bar{B}-B+1)e^{-\bar{B}} \ldots \right]$$

with $\lambda = e^{i\underline{\omega}t} \exp - \frac{1}{2} \sum_j r[\dot{x}_j(t) - \dot{x}_j(0)]^2$.

Thus, applying the transformation to the Gaussian velocity distribution

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[†] See Appendix A.

$$(6.8) \qquad e^{-\beta\phi(\dot{x}(0))} = e^{-\sum_j \frac{1}{2} m \dot{x}_j^2(0)}$$

$$(6.9) = \exp - \sum_j \frac{1}{2} m\beta[\sum_k \frac{1}{\sqrt{M}} e^{2\pi ijk/M} \dot{x}(k,0)]^2$$

$$= \exp - \frac{1}{2} m\beta \sum_{j,k,k'} \frac{1}{M} e^{2\pi ijk/M} e^{2\pi ijk'/M} \dot{x}(k,0)\dot{x}(k',0)$$

$$= \exp - \frac{1}{2} m\beta \sum_{k,k'} \delta_{k,-k'} \dot{x}(k,0)\dot{x}(k',0)$$

$$(6.10) = \exp - \frac{1}{2} \sum_k m\beta\dot{x}(k,0)\dot{x}(-k,0)$$

B for the path is $\beta\phi(\dot{x}(0)) + \beta\phi(x(0))$

$$- i \int_0^t \sum_j \xi_j(t')(\dot{x}_j(t') - \dot{x}_j(0))\, dt'$$

$$- \frac{i}{m} \int_{-\infty}^{0} \int_{-\infty}^{t'} \sum_s \xi_s(t')\, f_s(x(t''))\, dt'\, dt'' \qquad \text{for } t' < 0$$

$$- \frac{i}{m} \int_0^t \int_{-\infty}^{0} \sum_s \xi_s(t')\, f_s(x(t''))\, dt'\, dt'' \qquad \text{for } t' > 0$$

$$(6.11) \quad - \frac{i}{m} \int_0^t \int_0^{t'} \sum_s \xi_s(t')\, f_s(x(t''))\, dt'\, dt'' \qquad \text{for } t' > 0$$

where its potential is given by

$$(6.12) \quad \phi(x) = \sum_{s,j} \frac{1}{4} \tilde{A}_{sj}(x_s-x_j)^4 - \sum_{s,j} \frac{1}{2} m\tilde{\Omega}^2_{sj}(x_s-x_j)^2.$$

The purely quartic part in the mode variables will be turned on slowly from $t = -\infty$ to 0 via $e^{\gamma t}$ while the harmonic part of the quartic interaction arising from the normal mode transformation will be lumped with the ordinary harmonic term.

Hence, applying (6.3)-(6.5) one may write B in obvious notation as

$$(6.13)\quad \frac{1}{2}\sum_{j} m\beta[\sum_{k}\frac{1}{\sqrt{M}}e^{2\pi ijk/M}\dot{x}(k,0)]^{2}$$

$$+\beta e^{\gamma t}\sum_{s,j}\frac{1}{4}\tilde{A}_{sj}[\sum_{k}(e^{2\pi isk/M}-e^{2\pi ijk/M})\frac{x(k,0)}{\sqrt{M}}+(s-j)]^{4}$$

$$-\frac{1}{2}\beta\sum_{s,j}m\tilde{\Omega}^{2}_{sj}[\sum_{k}(e^{2\pi isk/M}-e^{2\pi ijk/M})\frac{x(k,0)}{\sqrt{M}}+(s-j)]^{2}$$

$$-i\int_{0}^{t}\sum_{j}(\sum_{k}\frac{1}{\sqrt{M}}e^{2\pi ijk/M}\xi(k,t'))(\sum_{k'}\frac{1}{\sqrt{M}}e^{2\pi ijk'/M}(\dot{x}(k',t')-\dot{x}(k,0))\,dt'$$

$$+\frac{i}{m}\int_{-\infty}^{0}\int_{-\infty}^{t'}\sum_{s}(\sum_{k}\frac{1}{\sqrt{M}}e^{2\pi isk/M}\xi(k,t'))(\sum_{j}\tilde{A}_{sj}[\sum_{k'}(e^{2\pi isk'/M}-e^{2\pi ijk'/M})$$

$$\cdot\frac{x(k',t'')}{\sqrt{M}}+(s-j)]^{3}-\sum_{j}m\tilde{\Omega}^{2}_{sj}[\sum_{k'}(e^{2\pi isk'/M}-e^{2\pi ijk'/M})\frac{x(k',t'')}{\sqrt{M}}$$

$$+(s-j)])\,dt'\,dt''+\frac{i}{m}\int_{0}^{t}\int_{-\infty}^{0}\dots+\frac{i}{m}\int_{0}^{t}\int_{0}^{t'}\dots$$

while $\overline{B}$ is given by

$$(6.14)\quad \frac{1}{2}\sum_{j}m\beta[\sum_{k}\frac{1}{\sqrt{M}}e^{2\pi ijk/M}\dot{x}(k,0)]^{2}+\frac{1}{2}\sum_{s,j}A_{sj}\beta(\sum_{k}[e^{2\pi isk/M}$$

$$-e^{2\pi ijk/M}]\frac{x(k,0)}{\sqrt{M}}+(s-j))^{2}-i\int_{0}^{t}\sum_{j}(\sum_{k}\frac{1}{\sqrt{M}}e^{2\pi ijk/M}\xi(k,t'))$$

$$\cdot(\sum_{k'}\frac{1}{\sqrt{M}}e^{2\pi ijk'/M}\{\dot{x}(k',t')-\dot{x}(k',0)\})\,dt'-\frac{i}{m}\int_{0}^{t}\int_{0}^{t'}\sum_{s,j}(\sum_{k}\frac{1}{\sqrt{M}}$$

$$\cdot e^{2\pi isk/M}\xi(k,t'))(A_{sj}\sum_{k'}\frac{1}{\sqrt{M}}e^{2\pi ijk'/M}x(k',t''))\,dt'\,dt''\,.$$

The simplification of $\overline{B}-B+1$ proceeds as follows. The term

$$(6.15)\quad \frac{1}{2}\beta\sum_{s,j}m\tilde{\Omega}^{2}_{sj}(\sum_{k}[e^{2\pi isk/M}-e^{2\pi ijk/M}]\frac{x(k,0)}{\sqrt{M}}+(s-j))^{2}$$

reduces to

$$(6.16) \qquad \sum_k m\beta\, e^{\pm 2\pi i k/M}\, \Omega^2 x(k,0)x(-k,0)$$

(where

$$\sum_{s,j} \frac{m\tilde{\Omega}^2_{sj}}{M}\, e^{2\pi i k j/M}\, e^{-2\pi i k s/M} = m\Omega^2),$$

and a linear term of the form

$$(6.17) \qquad \frac{1}{2} \sum_k m\beta\sqrt{M}\, \Omega^2\, e^{2\pi i k s/M}\, x(k,0) \quad ^{\dagger}$$

together with its symmetric counterpart in -k.

Skipping for a moment the third and fourth power terms,

$$(6.18) \quad -\frac{i}{m} \int_0^t \int_0^{t'} \sum_{s,j} \Big(\sum_k \frac{1}{\sqrt{M}}\, e^{2\pi i s k/M}\, \xi(k,t')\Big)\Big(A_{sj} \sum_{k'} \frac{1}{\sqrt{M}}\, e^{2\pi i j k'/M} \cdot x(k',t'')\Big)\, dt'\, dt''$$

becomes

$$(6.19) \quad -\frac{i}{m} \int_0^t \int_0^{t'} \sum_{\substack{s,j\\k,k'}} \frac{A_{sj}}{M}\, e^{2\pi i s k/M}\, e^{2\pi i j k'/M}\, \xi(k,t')x(k',t'')dt'dt''$$

$$(6.20) \quad = -i \sum_k \int_0^t \int_0^{t'} \omega^2 \xi(k,t')x(-k,t'')\, dt'\, dt''$$

i.e.

$$\sum_{s,j} \frac{A_{sj}}{M}\, e^{2\pi i k j/M}\, e^{-2\pi i k s/M} = m\omega^2 .$$

The third order term

[†] In demonstrating that the frequency shift goes to zero finite terms such as these are found in the denominator of the expression for Ω^2 (see Appendix D.III or equation (5.19)) and as time becomes infinite are, in comparison with the secular terms, of no consequence.

$$(6.21)\quad \sum_{s,j,k} \frac{\tilde{A}_{sj}}{\sqrt{M}}\, \xi(k,t')\, e^{2\pi isk/M} \Big(\sum_{k'} [e^{2\pi isk'/M} - e^{2\pi ijk'/M}] \cdot \frac{x(k',t'')}{\sqrt{M}} + (s-j)\Big)^3$$

$$= \sum_{s,j,k} \frac{\tilde{A}_{sj}}{\sqrt{M}}\, \xi(k,t')\, e^{2\pi isk/M} \Big(\{\sum_{k'} [e^{2\pi isk'/M} - e^{2\pi ijk'/M}] \frac{x(k',t'')}{\sqrt{M}}$$

$$+ (s-j)\}\{\sum_{k''} [e^{2\pi isk''/M} - e^{2\pi ijk''/M}] \frac{x(k'',t'')}{\sqrt{M}} + (s-j)\}$$

$$\cdot\{\sum_{k'''} [e^{2\pi isk'''/M} - e^{2\pi ijk''/M}] \frac{x(k''',t'')}{\sqrt{M}} + (s-j)\}\Big)$$

simplifies to

$$(6.22)\quad \sum_{\substack{s,j,k\\ k',k'',k'''}} e^{\gamma t''} \frac{\tilde{A}_{sj}}{M^2}\, \xi(k,t')x(k',t'')x(k'',t'')x(k''',t'')e^{2\pi isk/M}$$

$$\cdot\{e^{2\pi\frac{i}{M}(sk'+sk''+sk''')} - e^{2\pi\frac{i}{M}(jk'+sk''+sk''')}$$

$$-e^{2\pi\frac{i}{M}(sk'+jk''+sk''')} + e^{2\pi\frac{i}{M}(jk'+jk''+sk''')}$$

$$-e^{2\pi\frac{i}{M}(sk'+sk''+jk''')} + e^{2\pi\frac{i}{M}(jk'+sk''+jk''')}$$

$$+e^{2\pi\frac{i}{M}(sk'+jk''+jk''')} - e^{2\pi\frac{i}{M}(jk'+jk''+jk''')}\}$$

Once again odd powers in x are discarded (recall ξ contains x explicitly) and second power even terms will be lumped with the harmonic contribution. Hence, in like respect the fourth order term

$$(6.23)\quad \sum_{s,j} \frac{1}{4}\, \beta\, \tilde{A}_{sj} [\sum_{k}(e^{2\pi isk/M} - e^{2\pi ijk/M}) \frac{x(k,0)}{\sqrt{M}} + (s-j)]^4$$

is expressible as

$$(6.24)\quad \sum_{\substack{s,j,k'\\ k'',k''',k''''}} e^{\gamma t}\,\frac{1}{4}\,\beta\,\frac{\tilde{A}_{sj}}{M^2}\,x(k',0)x(k'',0)x(k''',0)x(k'''',0)$$

$$\cdot\{e^{2\pi\frac{i}{M}(sk'+sk''+sk'''+sk'''')} - e^{2\pi\frac{i}{M}(jk'+sk''+sk'''+sk'''')}$$

$$-e^{2\pi\frac{i}{M}(sk'+jk''+sk'''+sk'''')} + e^{2\pi\frac{i}{M}(jk'+jk''+sk'''+sk'''')}$$

$$-e^{2\pi\frac{i}{M}(sk'+sk''+jk'''+sk'''')} + e^{2\pi\frac{i}{M}(jk'+sk''+jk'''+sk'''')}$$

$$+e^{2\pi\frac{i}{M}(sk'+jk''+jk'''+sk'''')} - e^{2\pi\frac{i}{M}(jk'+jk''+jk'''+sk'''')}$$

$$-e^{2\pi\frac{i}{M}(sk'+sk''+sk'''+jk'''')} + e^{2\pi\frac{i}{M}(jk'+sk''+sk'''+jk'''')}$$

$$+e^{2\pi\frac{i}{M}(sk'+jk''+sk'''+jk'''')} - e^{2\pi\frac{i}{M}(jk'+jk''+sk'''+jk'''')}$$

$$+e^{2\pi\frac{i}{M}(sk'+sk''+jk'''+jk'''')} - e^{2\pi\frac{i}{M}(jk'+sk''+jk'''+jk'''')}$$

$$-e^{2\pi\frac{i}{M}(sk'+jk''+jk'''+jk'''')} + e^{2\pi\frac{i}{M}(jk'+jk''+jk'''+jk'''')}\}$$

The kernel

$$(6.25)\quad \exp -\frac{1}{2m\beta}\Big[\int_0^t\int_0^{t'} \sum_j\Big(\sum_k \frac{1}{\sqrt{M}}\, e^{2\pi ijk/M}\,\xi(k,t')\Big)\Big(\sum_{k'} \frac{1}{\sqrt{M}}\, e^{2\pi ijk'/M}$$

$$\cdot\,\xi(k',t'')\Big)dt'dt'' - ir\int_0^t \sum_j\Big(\sum_k \frac{1}{\sqrt{M}}\, e^{2\pi ijk/M}\,\dot{x}(k,t)\Big)\Big(\sum_{k'} \frac{1}{\sqrt{M}}$$

$$\cdot\, e^{2\pi ijk'/M}\,\xi(k',t')\,dt' - \frac{1}{4}\,r^2\sum_j\Big(\sum_k \frac{1}{\sqrt{M}}\, e^{2\pi ijk/M}\,\dot{x}(k,t)\Big)\Big(\sum_{k'} \frac{1}{\sqrt{M}}$$

$$\cdot\, e^{2\pi ijk'/M}\,\dot{x}(k',t)\Big]\ \exp -\frac{1}{2}\sum_{s,j}\beta\,A_{sj}\Big(\sum_k\big[e^{2\pi isk/M}-e^{2\pi ijk/M}\big]$$

$$\cdot\,\frac{x(k,0)}{M}\Big)^2\ \exp i\int_0^t \sum_j\Big(\sum_k \frac{1}{\sqrt{M}}\, e^{2\pi ijk/M}\,\xi(k,t')\Big)$$

$$\cdot\Big(\sum_{k'} \frac{1}{\sqrt{M}}\, e^{2\pi ijk'/M}\ \dot{x}(k',t')dt'\Big) \exp \frac{i}{m}\int_0^t\int_0^{t'} \sum_{s,j}\Big(\sum_k \frac{1}{\sqrt{M}}$$

$$\cdot e^{2\pi isk/M}\ \xi(k,t')\Big)\Big(A_{sj} \sum_{k'} \frac{1}{\sqrt{M}}\, e^{2\pi ijk'/M}\ x(k',t'')\Big)dt'\ dt''$$

becomes

$$(6.26)\quad \exp - \frac{1}{2m\beta}\Big[\int_0^t\int_0^{t'} \sum_{k,k'} \delta_{k,-k'}\ \xi(k,t')\xi(k',t'')dt'\ dt''$$

$$- ir\int_0^t \sum_{k,k'} \delta_{k,-k'}\ \dot{x}(k,t)\xi(k',t')dt'$$

$$- \frac{1}{4} r^2 \sum_{k,k'} \delta_{k,-k'}\ \dot{x}(k,t)\dot{x}(k',t')\Big]$$

$$\cdot e^{-m\beta\sum_k e^{\pm 2\pi ik/M}\ \omega^2 x(k,0)x(-k,0)}\ e^{i\int_0^t \sum_{k,k'} \xi(k,t')\dot{x}(k',t')dt'}$$

$$\cdot e^{i/m\int_0^t\int_0^{t'} \sum_k m\omega^2\ \xi(k,t')x(-k,t'')dt'dt''}$$

or finally

$$(6.27)\quad \exp - \frac{1}{2m\beta}\sum_k \Big[\int_0^t\int_0^{t'} \xi(k,t')\xi(-k,t'')\ dt'\ dt''$$

$$- ir\int_0^t \dot{x}(k,t)\xi(-k,t')\ dt' - \frac{1}{4} r^2\dot{x}(k,t)\dot{x}(-k,t)\Big]$$

$$\cdot\ e^{-m\beta\sum_k e^{\pm 2\pi ik/M}\ \omega^2 x(k,0)x(-k,0)}$$

$$\cdot\ e^{i\sum_k\int_0^t \xi(k,t')\dot{x}(-k,t')\ dt'}$$

$$\cdot\ e^{i\sum_k\int_0^t\int_0^{t'} \omega^2\xi(k,t')x(-k,t'')dt'dt''}\ ,$$

where the kernel is equally symmetric in k and -k.

B. Establishment of Inequalities

The full inequality is

$$(6.28) \qquad \int \lambda\, e^{-B} \geq \int \lambda(\bar{B}-B+1)\, e^{-\bar{B}}$$

$$(6.29) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp - \frac{1}{2m\beta} \sum_k \Big[\int_0^t \int_0^{t'} \xi(k,t')\xi(-k,t'')\, dt'\, dt''$$

$$- ir \int_0^t \dot{x}(k,t)\xi(-k,t')dt' - \frac{1}{4} r^2 \dot{x}(k,t)\dot{x}(-k,t)\Big]$$

$$\cdot\, e^{-m\beta \sum_k e^{\pm 2\pi ik/M} \omega^2 x(k,0)x(-k,0)}$$

$$\cdot\, e^{i \sum_k \int_0^t \xi(k,t')\dot{x}(-k,t')dt'}\; e^{\frac{i}{m} \sum_k \int_0^t \int_0^{t'} m\omega^2 \xi(k,t')x(-k,t'')dt'dt''}$$

$$\cdot\Big(1 + \frac{1}{2} \sum_{s,j} A_{sj}\beta\Big[\sum_k \left(e^{2\pi isk/M} - e^{2\pi ijk/M}\right)\frac{x(k,0)}{\sqrt{M}} + (s-j)\Big]^2$$

$$+ \frac{1}{4} \sum_{s,j} \beta\, \tilde{A}_{sj}\Big[\sum_k \left(e^{2\pi isk/M} - e^{2\pi ijk/M}\right)\frac{x(k,0)}{\sqrt{M}} + (s-j)\Big]^2$$

$$- \frac{1}{2} \sum_{s,j} m\beta\tilde{\Omega}^2_{sj}\Big[\sum_k \left(e^{2\pi isk/M} - e^{2\pi ijk/M}\right)\frac{x(k,0)}{\sqrt{M}} + (s-j)\Big]^2$$

$$- \frac{i}{m} \int_0^t \int_0^{t'} \sum_{s,j} \Big(\sum_k \frac{1}{\sqrt{M}} e^{2\pi isk/M}\, \xi(k,t')\Big)\Big(A_{sj} \sum_{k'} \frac{1}{\sqrt{M}} e^{2\ ijk'/M}$$

$$\cdot\, x(k',t'')\Big)dt'dt'' - \frac{i}{m} \int_{-\infty}^{0} \int_{-\infty}^{t'} e^{\gamma t''} \sum_s \Big(\sum_k \frac{1}{\sqrt{M}} e^{2\pi isk/M}\, \xi(k,t')\Big)$$

$$\cdot\Big(\sum_j \tilde{A}_{sj}\Big[\sum_{k'} \left(e^{2\pi isk'/M} - e^{2\pi ijk'/M}\right)\frac{x(k',t'')}{\sqrt{M}} + (s-j)\Big]^3 -$$

$$- \sum_{j} m\tilde{\Omega}^2_{sj}[\sum_{k'} (e^{2\pi isk'/M} - e^{2\pi ijk'/M}) \frac{x(k',t'')}{\sqrt{M}} + (s-j)])dt'dt''$$

$$- \frac{i}{m} \int_0^t \int_{-\infty}^0 \ldots - \frac{i}{m} \int_0^t \int_0^{t'} \ldots \prod_0^t d\xi(t')\, dx(t') \, .$$

After a good deal of tedious algebra[†] the inequality can be written

$$(6.30) \quad \int \lambda e^{-B} \ldots \geq \int \lambda(\bar{B}-B+1)e^{-\bar{B}} \ldots$$

$$= \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} \exp [- \frac{1}{2} \sum_{k} (c_{11}(k)x^2(k,0) + 2c_{12}(k)x(k,0)x(k,t)$$

$$+ c_{22}(k)x^2(k,t))](1+ \sum_{k} m\beta e^{\pm 2\pi ik/M} (\omega^2+\Omega^2)x(k,0)x(-k,0)$$

$$- \sum_{\substack{s,j,k\\k',k'',k'''}} \frac{1}{4} \beta\psi(s,j,k,k',k'',k''') \, x(k,0)x(k',0)x(k'',0)x(k''',0)$$

$$+\sum_{k} [m\beta(x(k,t)x(-k,t)-x(k,0)x(-k,t)\cos \omega t)\psi(s,j,k,k',k'',k''')$$

$$\cdot(b_1(t)+1)+ m\beta(x(-k,0)x(k,t)-x(-k,0)x(k,0)\cos \omega t)$$

$$\cdot\psi(s,j,k,k',k'',k''')(b_2(t)+1)+ \frac{1}{2} r(x(-k,t)x(k,t)\cos \omega t$$

$$- x(k,0)x(-k,t))(b_3(t))+ \frac{1}{2} r(x(-k,0)x(k,t)\cos \omega t$$

$$- x(-k,0)x(k,0))(b_4(t))] + \sum_{s,j,k,k',k'',k'''} \theta(s,j,k,k',k'',k''')$$

$$\cdot\{[x(k,t)x(-k',t)x(-k'',t)x(-k''',t)][a_1(t)] +$$

[†] See Appendix D.

$$+ [x(k,t)x(-k',0)x(-k'',0)x(-k''',0)][a_2(t)]+[x(k,t)x(-k',0)$$

$$\cdot x(-k'',t)x(-k''',t)+ x(k,t)x(-k',t)x(-k'',0)x(-k''',t)$$

$$+x(k,t)x(-k',t)x(-k'',t)x(-k''',0)][a_3(t)]+ [x(k,t)x(-k',0)$$

$$\cdot x(-k'',0)x(-k''',t)+ x(k,t)x(-k',0)x(-k'',t)x(-k''',0)$$

$$+x(k,t)x(-k',t)x(-k'',0)x(-k''',0)][a_4(t)]- [x(k,0)x(-k',t)$$

$$\cdot x(-k'',t)x(-k''',t)][a_5(t)]- [x(k,0)x(-k',0)x(-k'',0)x(-k''',0)]$$

$$\cdot [a_6(t)]- [x(k,0)x(-k',0)x(-k'',t)x(-k''',t)+x(k,0)x(-k',t)$$

$$\cdot x(-k'',0)x(-k''',t)+ x(k,0)x(-k',t)x(-k'',t)x(-k''',0)][a_7(t)]$$

$$-[x(k,0)x(-k',0)x(-k'',0)x(-k''',t)+ x(k,0)x(-k',0)x(-k'',t)$$

$$\cdot x(-k''',0)+ x(k,0)x(-k',t)x(-k'',0)x(-k''',0)][a_8(t)]\}$$

$$- \sum_k \Omega^2(e^{\pm 2\pi ik/M} -1)[\{m\beta(x(k,t)x(-k,t)- x(k,0)x(-k,t)\cos \omega t)$$

$$+ \frac{1}{2} r(x(k,t)x(-k,t)\cos \omega t - x(k,0)x(-k,t)\}\{c_1(t)\}$$

$$+ \{m\beta(x(k,t)x(-k,0)- x(k,0)x(-k,0)\cos \omega t)+ \frac{1}{2} r(x(k,t)$$

$$\cdot x(-k,0) \cos \omega t - x(k,0)x(-k,0)\}\{c_2(t)\}] D[\ldots] ;$$

where in the kernel the summation over k stands for k, k', k'', k''' terms and plus or minus values; moreover, $D[\ldots]$ means in each summation group one integrates over the appropriate $dx(k,0)$ or $dx(k'',t)$ whatever the case may be. Such terms as $c_{11}(k)$, $c_{12}(k)$, $c_{22}(k)$, $\psi(s,j,k,k',k'',k''')$, $b_1(t)$, $b_2(t)$, $b_3(t)$, $b_4(t)$, $\theta(s,j,k,k',k'',k''')$, $a_1(t)$, $a_2(t)$, $a_3(t)$, $a_4(t)$, $a_5(t)$, $a_6(t)$, $a_7(t)$, $a_8(t)$, $c_1(t)$ and $c_2(t)$ will be identified, but first some of the terms leading to this inequality are clarified. The combined three third order terms including the phase

$$(6.31)\quad -\frac{i}{m}\int_{-\infty}^{0} dt' \int_{-\infty}^{t'} dt''\, e^{\gamma t''} \sum_s \Big[\sum_k \frac{1}{\sqrt{M}} e^{2\pi i s k/M}\, \xi(k,t')\Big)$$

$$\cdot\Big(\sum_j \tilde{A}_{sj}\Big[\sum_{k'} \big(e^{2\pi i s k'/M} - e^{2\pi i j k'/M}\big)\frac{x(k',t'')}{\sqrt{M}} + (s-j)\Big]^3$$

$$-\frac{i}{m}\int_0^t \int_{-\infty}^0 \cdots - \frac{i}{m}\int_0^t \int_0^{t'} \cdots$$

are reducible to

$$(6.32)\quad \sum_{\substack{s,j,k\\k',k'',k'''}} \frac{\tilde{A}_{sj}}{M^2}\Big\{e^{2\pi i\frac{s}{M}(k+k'+k''+k''')} - e^{2\pi\frac{i}{M}(jk'+sk''+sk'''+sk)}$$

$$-e^{2\pi\frac{i}{M}(sk+sk'+jk''+sk''')} + e^{2\pi\frac{i}{M}(sk+jk'+jk''+sk''')}$$

$$-e^{2\pi\frac{i}{M}(sk+sk'+sk''+jk''')} + e^{2\pi\frac{i}{M}(sk+jk'+sk''+jk''')}$$

$$+e^{2\pi\frac{i}{M}(sk+sk'+jk''+jk''')} - e^{2\pi\frac{i}{M}(sk+jk'+jk''+jk''')}\Big\}\,.$$

$$\cdot\{\frac{\beta(x(k,t)-x(k,0)\cos\omega t)}{\sin^5\omega t} + \frac{r}{2m}(\frac{x(k,t)\cos\omega t-x(k,0)}{\sin^5\omega t})\}$$

$$\cdot\{[x(-k',t)x(-k'',t)x(-k''',t)][-\frac{3}{8}\frac{\omega}{\gamma}\cos\omega t+\frac{19}{96}\sin\omega t$$

$$-\frac{2}{3}\sin\omega t+\frac{45}{96}\sin\omega t+\frac{\sin 4\omega+\cos\omega t}{96}+\frac{5\sin\omega\omega t\cos 2\omega t}{24}$$

$$-\frac{\sin\omega t\cos 4\omega t}{96}-\frac{\cos\omega t\sin 2\omega t}{6}]+[x(-k',0)x(-k'',0)x(-k''',0)]$$

$$\cdot[\frac{3}{8}\frac{\omega\cos\omega t}{\gamma}+\frac{\sin 4\omega t}{96}-\frac{\sin 2\omega t}{6}-\frac{1}{3}\sin^3\omega t\cos\omega t+\frac{\sin 2\omega t}{3}$$

$$-\frac{\sin 4\omega t}{96}-\frac{\sin 2\omega t}{6}-\frac{\sin^3\omega t\cos\omega t}{3}+\frac{\sin 2\omega t}{3}]$$

$$+[x(-k',0)x(-k'',t)x(-k''',t)+x(-k',t)x(-k'',0)x(-k''',t)$$

$$+x(-k',t)x(-k'',t)x(-k''',0)][-\frac{11}{96}\sin 2\ t+\frac{1}{8}\frac{\omega\sin^2\omega t}{\gamma}$$

$$+\frac{3}{8}\frac{\omega\cos^2\omega t}{\gamma}+\frac{1}{3}\sin 2\omega t+\frac{\sin 2\omega t\cos 4\omega t}{96}-\frac{\sin^2\omega t\sin 2\omega t}{12}$$

$$+\frac{\sin^2\omega t\sin 4\omega t}{96}-\frac{\cos^2\omega t\sin 4\omega t}{96}+\frac{\cos^2\omega t\sin 2\omega t}{6}-\frac{\sin 4\omega t}{16}$$

$$-\frac{9}{32}\sin 2\omega t]+[x(-k',0)x(-k'',0)x(-k''',t)+x(-k',0)x(-k'',t)$$

$$\cdot x(-k''',0)+x(-k',t)x(-k'',0)x(-k''',0)][\frac{\sin\omega t\cos 2\omega t}{24}$$

$$-\frac{\sin\omega t\cos 4\omega t}{96}-\frac{3}{8}\frac{\omega\cos^2\omega t}{\gamma}-\frac{\cos\omega t\sin 4\omega t}{96}+\frac{\cos\omega t\sin 2\omega t}{6}$$

$$-\frac{\sin\omega t}{3}-\frac{\sin\omega t\cos^2\omega t}{3}+\frac{\sin\omega t}{12}-\frac{\sin\omega t\cos 2\omega t}{12}-$$

$$-\frac{\sin\omega t\sin 4\omega t}{96}+\frac{\cos\omega t\sin 4\omega t}{96}+\frac{\cos\omega t\sin 2\omega t}{6}$$

$$+\frac{\sin^3\omega t}{3}+\frac{2\sin\omega t\cos^2\omega t}{3}]\}$$

which with redefining the phase and simplifying becomes

$$
\begin{aligned}
(6.33)\quad & \sum_{\substack{s,j,k\\ k',k'',k'''}} \theta(s,j,k,k',k'',k''')\{[x(k,t)x(-k',t)x(-k'',t) \\
& \cdot x(-k''',t)][a_1(t)] + [x(k,t)x(-k',0)x(-k'',0)x(-k''',0)] \\
& \cdot [a_2(t)] + [x(k,t)x(-k',0)x(-k'',t)x(-k''',t) + x(k,t)x(-k',t) \\
& \cdot x(-k'',0)x(-k''',t) + x(k,t)x(-k',t)x(-k'',t)x(-k''',0)][a_3(t)] \\
& + [x(k,t)x(-k',0)x(-k'',0)x(-k''',t) + x(k,t)x(-k',0)x(-k'',t) \\
& \cdot x(-k''',0) + x(k,t)x(-k',t)x(-k'',0)x(-k''',0)][a_4(t)] \\
& - [x(k,0)x(-k',t)x(-k'',t)x(-k''',t)][a_5(t)] - [x(k,0)x(-k',0) \\
& \cdot x(-k'',0)x(-k''',0)][a_6(t)] - [x(k,0)x(-k',0)x(-k'',t) \\
& \cdot x(-k''',t) + x(k,0)x(-k',t)x(-k'',0)x(-k''',t) + x(k,0) \\
& \cdot x(-k',t)x(-k'',t)x(-k''',0)][a_7(t)] - [x(k,0)x(-k',0) \\
& \cdot x(-k'',0)x(-k''',t) + x(k,0)x(-k',0)x(-k'',t)x(-k''',0) \\
& + x(k,0)x(-k',t)x(-k'',0)x(-k''',0)][a_8(t)]\}.
\end{aligned}
$$

Likewise the fourth order term may be rewritten as well, and since all summation indices are merely dummy, one may let $k' \to k$; $k'' \to k'$; $k''' \to k''$; $k'''' \to k'''$ which makes this term notationally compatible with the third order terms.

$$
(6.34)\quad \sum_{s,j} \frac{1}{4}\beta \tilde{A}_{sj}\Big[\sum_{k}\big(e^{2\pi isk/M} - e^{2\pi ijk/M}\big)\frac{x(k,0)}{\sqrt{M}} + (s-j)\Big]^4
$$

$$
(6.35)\quad = \sum_{\substack{s,j,k\\ k',k'',k'''}} \frac{1}{4}\beta\psi(s,j,k,k',k'',k''')x(k,0)x(k',0)x(k'',0) \cdot x(k''',0)
$$

where

$$
\begin{aligned}
(6.35)' \quad \theta(s,j,k,k',k'',k''') = \frac{\tilde{A}_{sj}}{M^2} \{ & e^{2\pi i\frac{s}{M}(k+k'+k''+k''')} \\
& -e^{2\pi\frac{i}{M}(jk'+sk''+sk'''+sk)} - e^{2\pi\frac{i}{M}(sk+sk'+jk''+sk''')} \\
& +e^{2\pi\frac{i}{M}(sk+jk'+jk''+sk''')} - e^{2\pi\frac{i}{M}(sk+sk'+sk''+jk''')} \\
& +e^{2\pi\frac{i}{M}(sk+jk'+sk''+jk''')} + e^{2\pi\frac{i}{M}(sk+sk'+jk''+jk''')} \\
& -e^{2\pi\frac{i}{M}(sk+jk'+jk''+jk''')} \}
\end{aligned}
$$

$$
\begin{aligned}
\psi(s,j,k,k',k'',k''') = \frac{\tilde{A}_{sj}}{M^2} \{ & e^{2\pi i\frac{s}{M}(k+k'+k''+k''')} \\
& -e^{2\pi\frac{i}{M}(jk+sk'+sk''+sk''')} - e^{2\pi\frac{i}{M}(sk+jk'+sk''+sk''')} \\
& +e^{2\pi\frac{i}{M}(jk+jk'+sk''+sk''')} - e^{2\pi\frac{i}{M}(sk+sk'+jk''+sk''')} \\
& +e^{2\pi\frac{i}{M}(jk+sk'+jk''+sk''')} + e^{2\pi\frac{i}{M}(sk+jk'+jk''+sk''')} \\
& -e^{2\pi\frac{i}{M}(jk+jk'+jk''+sk''')} - e^{2\pi\frac{i}{M}(sk+sk'+sk''+jk''')} \\
& +e^{2\pi\frac{i}{M}(jk+sk'+sk''+jk''')} + e^{2\pi\frac{i}{M}(sk+jk'+sk''+jk''')} \\
& -e^{2\pi\frac{i}{M}(jk+jk'+sk''+jk''')} + e^{2\pi\frac{i}{M}(sk+sk'+jk''+jk''')} \\
& -e^{2\pi\frac{i}{M}(jk+sk'+jk''+jk''')} - e^{2\pi\frac{i}{M}(sk+jk'+jk''+jk''')} \\
& +e^{2\pi\frac{i}{M}(jk+jk'+jk''+jk''')} \};
\end{aligned}
$$

$$
\begin{aligned}
a_1(t)\Big|_{r=0} = \frac{\beta}{\sin^5 \omega t} \Big(& \frac{3}{8}\,\frac{\omega \cos \omega t}{\gamma} + \frac{\sin 4\omega t \cos \omega t}{96} \\
& + \frac{5 \sin \omega t \cos 2\omega t}{24} - \frac{\sin \omega t \cos 4\omega t}{96} - \frac{\cos \omega t \sin 2\omega t}{6} \Big)
\end{aligned}
$$

$$
a_2(t)\Big|_{r=0} = \frac{\beta}{\sin^5 \omega t} \left(\frac{3\omega \cos^2 \omega t}{8\gamma} + \frac{\sin 2\omega t}{3} \right)
$$

$$a_3(t)\Big|_{r=0} = \frac{\beta}{\sin^5\omega t}\Big(-\frac{\sin 2\omega t}{16} - \frac{\sin 4\omega t}{16} - \frac{3}{8}\,\frac{\omega\cos^2\omega t}{\gamma}$$

$$+ \frac{\sin 2\omega t\cos 4\omega t}{96} - \frac{\cos 2\omega t\sin 4\omega t}{96} - \frac{\sin^2\omega t\sin 2\omega t}{12}$$

$$+ \frac{\cos^2\omega t\sin 2\omega t}{6}\Big)$$

$$a_4(t)\Big|_{r=0} = \frac{\beta}{\sin^5\omega t}\Big(-\frac{\sin\omega t}{12} - \frac{\sin\omega t\cos 2\omega t}{24} - \frac{\sin\omega t\cos 4\omega t}{96}$$

$$- \frac{\sin\omega t\sin 4\omega t}{96} - \frac{3\omega\cos^2\omega t}{8} + \frac{\cos\omega t\sin 2\omega t}{3} + \frac{\cos\omega t\sin 4\omega t}{96}\Big)$$

$$a_5(t)\Big|_{r=0} = -\frac{\beta\cos\omega t}{\sin^5\omega t}\Big(-\frac{3\omega\cos\omega t}{8\gamma} + \frac{\sin 4\omega t\cos\omega t}{96}$$

$$+ \frac{5\sin\omega t\cos 2\omega t}{24} - \frac{\sin\omega t\cos 4\omega t}{96} - \frac{\cos\omega t\sin 2\omega t}{6}\Big)$$

$$a_6(t)\Big|_{r=0} = -\frac{\beta\cos\omega t}{\sin^5\omega t}\Big(\frac{3\omega}{8\gamma} + \frac{\sin 2\omega t}{3}\Big)$$

$$a_7(t)\Big|_{r=0} = -\frac{\beta\cos\omega t}{\sin^5\omega t}\Big(-\frac{\sin 2\omega t}{16} - \frac{\sin 4\omega t}{16} - \frac{3\omega\cos\omega t}{8}$$

$$+ \frac{\sin 2\omega t\cos 4\omega t}{96} - \frac{\cos 2\omega t\sin 4\omega t}{96} - \frac{\sin^2\omega t\sin 2\omega t}{12}$$

$$+ \frac{\cos^2\omega t\sin 2\omega t}{6}\Big)$$

$$a_8(t)\Big|_{r=0} = -\frac{\beta\cos\omega t}{\sin^5\omega t}\Big(\frac{\sin\omega t}{12} - \frac{\sin\omega t\cos 2\omega t}{24} -$$

$$- \frac{\sin\omega t\cos 4\omega t}{96} - \frac{\sin\omega t\sin 4\omega t}{96} - \frac{3\omega\cos\omega t}{8\gamma}$$

$$+ \frac{\cos\omega t\sin 2\omega t}{3} + \frac{\cos\omega t\sin 4\omega t}{96}\Big)$$

to get the $a_i(t)$ with $r \neq 0$ let $\beta \to \beta + \frac{r}{2m}\cos\omega t$ for $i = 1,2,3,4$ and $\beta\cos\omega t \to \beta\cos\omega t + \frac{r}{2m}$ for $i = 5,6,7,8$.

$$b_1(t) = b_3(t) = c_1(t) = \frac{1}{2\omega}\sin\omega t - \frac{1}{2}\, t \cos\omega t$$

$$b_2(t) = b_4(t) = c_2(t) = \frac{1}{2}\, t - \frac{1}{2}\, t\cos\omega t + \frac{1}{4\omega}\sin 2\omega t - \frac{1}{2\omega}\sin\omega t .$$

C. N-Body Renormalization Procedure

It is to be observed that expression (6.30) has a structure somewhat akin to equation (5.14) and therefore it is reasonable to expect that a similar method for renormalization of divergences can be employed.[†] In actuality, however, renormalization will not be accomplished by way of the frequency shifted harmonic terms but instead by their square. At first, it would appear that such a procedure alters drastically the variationally derived equations of motion, but it will be shown that the only change is a scaling of frequency. The integrand of the inequality is of the form

$$(F_1 - \Delta F)\, e^{(F_0 - F_1)}$$

where

F_0 is the basic harmonic oscillator term

ΔF is any perturbation term

F_1 is a shifted harmonic term.

Furthermore, by choosing $G^2 = F_1$ one can write

$$e^{F_0 - G^2} = \int e^{2i\lambda G}\, e^{-\lambda^2}\, e^{F_0}\, d\lambda$$

and so one has,

[†] Our initial approach was to integrate inequality (6.30), make the complex time extension, let time go to infinity, and then balance the various secular terms by their orders of infinity; this, however, was too tedious a procedure.

$$(6.36)\quad e^{F_0-G^2} = \exp -\frac{1}{2m\beta}\sum_k\Big[\int_0^t\int_0^{t'} \xi(k,t')\xi(-k,t'')\,dt'\,dt''$$

$$- ir\int_0^t \dot{x}(k,t)\xi(-k,t')\,dt' - \frac{1}{4}r^2\,\dot{x}(k,t)\dot{x}(-k,t)\Big]$$

$$\cdot\, e^{-m\beta\sum_k e^{\pm 2\pi ik/M}\,\omega^2 x(k,0)x(-k,0)}\; e^{i\sum_k\int_0^t \xi(k,t')\dot{x}(-k,t')dt'}$$

$$\cdot\, e^{-\{\sum_k\int_0^t\int_0^{t'}(-\Omega^2)\xi(k,t')x(-k,t'')dt'dt''\}^2}$$

$$\cdot\, e^{+i\sum_k\int_0^t\int_0^{t'}\omega^2\xi(k,t')x(-k,t'')dt'dt''}$$

$$(6.37)\quad = \int d\lambda\; e^{2i\lambda\{\sum_k\int_0^t\int_0^{t'}(\tilde{\omega}^2-\Omega^2)\xi(k,t')x(-k,t'')dt'dt''\}}\; e^{-\lambda^2}$$

$$\cdot\, e^{-m\beta\sum_k e^{\pm 2\pi ik/M}\,\omega^2 x(k,0)x(-k,0)}\; e^{i\sum_k\int_0^t \xi(k,t')\dot{x}(-k,t')dt'}$$

$$\cdot\exp -\frac{1}{2m\beta}\sum_k\Big[\int_0^t\int_0^{t'} \xi(k,t')\xi(-k,t'')\,dt'\,dt''$$

$$- ir\int_0^t \dot{x}(k,t)\xi(-k,t')\,dt' - \frac{1}{4}r^2\,\dot{x}(k,t)\dot{x}(-k,t)\Big]$$

where $i\omega^2 = 2i\lambda\tilde{\omega}^2$. After carrying through the variational technique one obtains the frequency scaled equations

$$\sum \ddot{x}(k,\tau) + 2\lambda(\tilde{\omega}^2-\Omega^2)x(k,\tau) = 0$$

$$\sum \ddot{\xi}(k,\tau) + 2\lambda(\tilde{\omega}^2-\Omega^2)x(k,\tau) = 0\ ,$$

and clearly the only change is a scaling of the frequency which leaves the calculation essentially unaltered. Following the methodology of Chapter V Section D one can again show that the frequencey shift term is zero† and the only finite contribution to the integral comes from various fourth power terms. This leads to a relatively simple inequality; hence, following the above outline one obtains upon integration[†] the finite contribution (for expression (6.30))

---

†See Appendix D.

$$(6.38)\quad \sum_k \left(-\frac{3\pi}{4}\right)\beta\psi(s,j,k,k,k,k)\Big[\frac{1}{[c_{11}(k)c_{22}(k)-c_{12}^2(k)]^{1/2}}\frac{\partial}{\partial r}$$

$$\cdot\,\frac{1}{c_{11}^2(k)}+\frac{c_{12}^2(k)}{[c_{11}(k)c_{22}(k)-c_{12}^2(k)]^{3/2}}\frac{\partial}{\partial r}\frac{1}{c_{11}^2(k)}$$

$$+\frac{c_{12}^4(k)}{[c_{11}(k)c_{22}(k)-c_{12}^2(k)]}\frac{\partial}{\partial r}\frac{1}{c_{11}^2(k)}$$

$$+\frac{2c_{12}(k)}{c_{11}^2(k)[c_{11}(k)c_{22}(k)-c_{12}^2(k)]^{3/2}}\frac{\partial}{\partial r}\left(c_{12}(k)-\frac{r\omega^2\cos^2\omega t}{2\sin^2\omega t}\right)$$

$$+\frac{4c_{12}^3(k)}{c_{11}^2(k)[c_{11}(k)c_{22}(k)-c_{12}^2(k)]^{5/2}}\frac{\partial}{\partial r}\left(c_{12}(k)-\frac{r\omega^2\cos^2\omega t}{2\sin^2\omega t}\right)\Big]\Bigg|_{\substack{r=0\\ t\to i\tau}}$$

$$(6.39)\quad =\sum_k\frac{3\pi\beta\psi(s,j,k,k,k,k)\omega^2\cosh\omega\tau}{2\beta^3m^3\omega^6\sinh^2\omega\tau\left(-e^{2\pi ik/M}+\frac{\cosh^2\omega\tau}{\sinh^2\omega\tau}\right)^3}$$

$$\cdot\Big[\left(\frac{\beta^2m^2\omega^4}{\sinh^2\omega\tau}\left[-e^{2\pi ik/M}+\frac{\cosh\omega\tau}{\sinh^2\omega\tau}-\frac{\cosh^2\omega\tau}{\sinh^2\omega\tau}\right]\right)^{-1/2}$$

$$+\beta^2m^2\omega^4\,\frac{\cosh^2\omega\tau}{\sinh^4\omega\tau}\left(\frac{\beta^2m^2\omega^4}{\sinh^2\omega\tau}\left[-e^{2\pi ik/M}+\frac{\cosh\omega\tau}{\sinh^2\omega\tau}-\frac{\cosh^2\omega\tau}{\sinh^2\omega\tau}\right]\right)^{-3/2}$$

$$+\beta^4m^4\omega^8\,\frac{\cosh^4\omega\tau}{\sinh^8\omega\tau}\left(\frac{\beta^2m^2\omega^4}{\sinh^2\omega\tau}\left[-e^{2\pi ik/M}+\frac{\cosh\omega\tau}{\sinh^2\omega\tau}-\frac{\cosh^2\omega\tau}{\sinh^2\omega\tau}\right]\right)^{-5/2}\Big]$$

$$-\sum_k\frac{3\pi\beta\psi(s,j,k,k,k,k)\cosh\omega\tau}{4\beta^4m^4\omega^6\sinh^4\omega\tau\left(-e^{2\pi ik/M}+\frac{\cosh^2\omega\tau}{\sinh^2\omega\tau}\right)^2}$$

[†] See Appendix D.

$$\cdot[(\frac{1}{\sinh^2\omega\tau}[-e^{2\pi ik/M}+\frac{\cosh\omega\tau}{\sinh^2\omega\tau}-\frac{\cosh^2\omega\tau}{\sinh^2\omega\tau}])^{-3/2}$$

$$+\frac{2\cosh^3\omega\tau}{\sinh^6\omega\tau}(\frac{1}{\sinh^2\omega\tau}[-e^{2\pi ik/M}+\frac{\cosh\omega\tau}{\sinh^2\omega\tau}-\frac{\cosh^2\omega\tau}{\sinh^2\omega\tau}])^{-5/2}]$$

where the $c_{ij}(k)$ are defined in Appendix C and as $\tau \to \infty$ this leaves

$$(6.40)\quad \sum_k \frac{3\pi\beta\psi(s,j,k,k,k,k)}{2\beta^4 m^4\omega^6(1-e^{2\pi ik/M})^3}[\frac{1}{(1+e^{2\pi ik/M})^{1/2}}-\frac{1}{(1+e^{2\pi ik/M})^{3/2}}$$

$$+\frac{1}{(1+e^{2\pi ik/M})^{5/2}}]-\sum_k \frac{3\pi\beta\psi(s,j,k,k,k,k)}{4\beta^4 m^4\omega^6(1-e^{2\pi ik/M})^2}$$

$$\cdot[-\frac{1}{(1+e^{2\pi ik/M})^{3/2}}+\frac{2}{(1+e^{2\pi ik/M})^{5/2}}]$$

since $\lim_{\tau\to\infty}\tanh\omega\tau \to 1$ and $\lim_{\tau\to\infty} 1/\sinh\omega\tau \to 0$.

Thus, the final form is[†]

$$(6.41)\quad \frac{\partial}{\partial r}\int \lambda\, e^{-B}\Big|_{\substack{\omega\to 0+\\ \bar{r}=0\\ \tau\to\infty}} \leq \frac{\partial}{\partial r}\int \lambda(\bar{B}-B+1)\, e^{-\bar{B}}\Big|_{\substack{\omega\to 0+\\ \bar{r}=0\\ \tau\to\infty}}$$

$$=\sum_k \frac{3\pi\psi(s,j,k,k,k,k)}{2m^4\beta^3\omega^6(1-e^{2\pi ik/M})^3}[\frac{1}{(1+e^{2\pi ik/M})^{1/2}}-\frac{1}{(1+e^{2\pi ik/M})^{3/2}}$$

$$+\frac{1}{(1+e^{2\pi ik/M})^{5/2}}]+\sum_k \frac{3\pi\psi(s,j,k,k,k,k)}{4m^4\beta^3\omega^6(1-e^{2\pi ik/M})^2}$$

$$\cdot[\frac{1}{(1+e^{2\pi ik/M})^{3/2}}-\frac{2}{(1+e^{2\pi ik/M})^{5/2}}]$$

[†] This is so because λ was taken as $\varepsilon^{i\omega t}\exp-\frac{1}{2}\sum_j r[\dot{x}_j(t)-\dot{x}_j(0)]^2$.

$$(6.42) = \sum_k \frac{3\pi\psi(s,j,k,k,k,k)}{128m\beta^3\gamma_1^3 \sin^6 \pi k/M} \quad \frac{1}{(1-e^{2\pi ik/M})^2}$$

$$\cdot \left[\frac{1}{(1-e^{2\pi ik/M})} \cdot \frac{1}{(1+e^{2\pi ik/M})^{1/2}}\right.$$

$$- \frac{1}{(1-e^{2\pi ik/M})} \cdot \frac{1}{(1+e^{2\pi ik/M})^{3/2}}$$

$$+ \frac{1}{(1-e^{2\pi ik/M})} \cdot \frac{1}{(1+e^{2\pi ik/M})^{5/2}}$$

$$\left. + \frac{1}{2(1+e^{2\pi ik/M})^{3/2}} - \frac{1}{(1+e^{2\pi ik/M})^{5/2}}\right]$$

where $\gamma_1 = \max\ (A_{sj})$.

CHAPTER VII

Throughout the development of the paper the scheme has been to determine the transport coefficient given the correlation function. This was accomplished essentially by the method of Kubo transforms. We now consider the hydrodynamic point of view. In order to do this we first review a paper of R. D. Mountain [20] where he calculates the spectral distribution of light scattered by density fluctuations in a dense, monatomic, one-component fluid from the time dependence of the density fluctuations predicted by the linearized hydrodynamic equations of irreversible thermodynamics.

A. Hydrodynamic Theory of Fluctuations

Information about the density fluctuations is contained in the generalized structure factor S(k,ω) which is the space and time Fourier transform of the two-body correlation function of the medium. The decay in time of density fluctuations is presumably described by the linearized hydrodynamic equations of irreversible thermodynamics, which are the continuity equation

$$(7.1) \qquad \frac{\partial \rho_1}{\partial t} + \rho_0 \operatorname{div} \underset{\sim}{v} = 0$$

the Navier-Stokes equation

$$(7.2) \quad \rho_0\, \partial \underset{\sim}{v}/\partial t + \frac{c_0^2}{\gamma} \operatorname{grad} \rho_1 + \frac{c_0^2 \beta \rho_0}{\gamma} \operatorname{grad} T_1 - (\tfrac{4}{3}\eta_s + \eta_B) \operatorname{grad} \operatorname{div} \underset{\sim}{v} = 0$$

and the energy-transport equation

$$(7.3) \qquad \rho_0 c_v \frac{\partial T_1}{\partial t} - \frac{c_v(\gamma-1)}{\beta} \frac{\partial \rho_1}{\partial t} - \lambda \nabla^2 T_1 = 0$$

In these equations, $\rho = \rho_0 + \rho_1$ is the number density, $T = T_0 + T_1$ is the temprature, ρ_0 and T_0 being the equilibrium values. The ratio of the specific heat at constant pressure to the specific heat at constant volume is given by $\gamma = c_p/c_v$. The shear and bulk viscosities are η_s and η_B, λ is the thermal conductivity, β is the thermal expansion coefficient, and c_0 is the low frequency limit of sound velocity. For this theory of small oscillations about equilibrium, the transverse part of the velocity is not coupled to the density. Thus, one can neglect the transverse part of the Navier-Stokes equation in all considerations. This limits the usability of this theory to fluids for which angular correlations between the molecules are not important.

To proceed one first eliminates the velocity by taking the divergence of each term in equation (7.2) and then substitutes for div $\underset{\sim}{v}$ from equation (7.1). Next one obtains the Fourier (space) and Laplace (time) transforms of these equations. Then one solves the resulting equations for n(k,s), the Fourier-Laplace transform of the density. The inverse Laplace transform of n(k,s) is the time-dependent, k-th Fourier component of the density, n(k,t):

$$(7.4) \qquad n(k,s) = \int_V dr \int_0^\infty dt \; e^{-ikr} \, e^{-st} \, \rho_1(r,t)$$

$$(7.4)' \quad T(k,s) = \int_V dr \int_0^\infty dt \; e^{-ikr} \, e^{-st} \, T_1(r,t) \; .$$

The elimination of the longitudinal component of velocity and the transformation of the density and temperature leads to two simultaneous linear equations for n(k,s) and T(k,s) in terms of the initial values

$$(7.5) \qquad n(k) = \int_V dr \; e^{-ikr} \, \rho_1(r,0)$$

$$(7.5)' \qquad T(k) = \int_V dr \; e^{-ikr} \, T_1(r,0) \; .$$

These equations are

$$(7.6) \; n(k,s)[s^2 + c_0^2 k^2/\gamma + (\tfrac{4}{3}\,\eta_s + \eta_B)k^2 s/\rho_0] + (c_0^2 \beta \rho_0 k^2/\gamma) T(k,s)$$
$$= n(k)[s + (\tfrac{4}{3}\,\eta_s + \eta_B)k^2/\rho_0]$$

and

$$(7.6)' \; n(k,s)[-sc_v(\gamma-1)/\beta] + T(k,s)[\rho_0 c_v s + \lambda k^2]$$
$$= -n(k)\; c_v(\gamma-1)/\beta + \rho_0 c_v \; T(k) \; .$$

The solution of equations (7.6) and (7.6)' for n(k,s) is

$$(7.7) \; n(k,s) = n(k) \frac{s^2 + (a+b)k^2 s + abk^4 + c_0^2(1-\gamma^{-1})k^2}{s^3 + (a+b)k^2 s^2 + (c_0^2 k^2 + abk^4)s + ac_0^2 k^4 \gamma^{-1}}$$

where $a = \lambda/\rho_0 c_v$ and $b = (\tfrac{4}{3}\,\eta_s + \eta_B)/\rho_0$.

The next step is to compute the inverse Laplace transform of n(k,s). This inversion requires that one find the roots of the denominator of equation (7.7), so

$$(7.8) \quad s^3 + (a+b)k^2 s^2 + (c_0^2 k^2 + abk^4)s + ac_0^2 k^4 \gamma^{-1} = 0$$

the solutions[†] of which to lowest order in ak^2 and bk^2 are

$$s = \pm c_0k - \frac{1}{2}(a+b-a\gamma^{-1})k^2$$

$$s = -(a/\gamma)k^2 \;;$$

or in terms of the original parameters

$$(7.8) \quad s = \pm ic_0k - \frac{1}{2}\left[\frac{\frac{4}{3}\eta_s+\eta_B}{\rho_0} + \frac{1}{\rho_0}\left(\frac{\lambda}{c_v} - \frac{\lambda}{c_p}\right)\right]k^2$$

$$(7.8)' \quad s = -\lambda k^2/\rho_0c_p \;.$$

The real part of the first two solutions is effectively the low-frequency sound-absorption coefficient and henceforth is denoted by Γk^2; viz.,

$$(7.9) \quad \Gamma k^2 = \frac{1}{2}\left[\frac{\frac{4}{3}\eta_s+\eta_B}{\rho_0} + \frac{1}{\rho_0}\left(\frac{\lambda}{c_v} - \frac{\lambda}{c_p}\right)\right]k^2 \;.$$

Using the first-order solutions, equations (7.8) and (7.8)', the lowest order terms of the inverse Laplace transform of $n(k,s)$ are

$$(7.10) \quad n(k,t) = n(k)\left\{\frac{c_p-c_v}{c_p}\exp\left[-\frac{\lambda k^2}{\rho_0c_p}t\right] + \frac{c_v}{c_p}\exp[-\Gamma k^2t]\cos c_0kt\right\}.$$

[†] In R. D. Mountain's paper he describes a convergent scheme to approximate the solutions to the dispersion equation (7.8) by using a power series with parameters ak^2/c_0k and bk^2/c_0k. These are of the order of 1/100 because typically in light scattering one has changes in the wave vector k of about 10^5cm^{-1} (this corresponds to a scattering angle of 60° when 6328Å He-Ne laser is used as the light source).

The k-th component of the density-density correlation function F(k,t) is

$$(7.11)\quad F(k,t) = \langle n(-k)n(k,t)\rangle$$

$$= \langle n(-k)n(k)\rangle\{\frac{c_p - c_v}{c_p}\exp[-\frac{\lambda k^2}{\rho_0 c_p}t] + \frac{c_v}{c_p}\exp[-\Gamma k^2 t]\cos c_0 kt\}.$$

The angular brackets <...> indicate an ensemble average over the initial values of the variables. The quantity which is of immediate interest in a light scattering experiment is the generalized structure factor $S(k,\omega)$;

$$(7.12)\qquad S(k,\omega) = 2\ \mathrm{Re}\int_0^\infty dt\ \exp\ (i\omega t)\ F(k,t)\ .$$

It follows from equation (7.11) that

$$S(k,\omega) = s(k)\ \sigma(k,\omega)\ ,$$

where $\qquad S(k) = \langle n(-k)n(k)\rangle$

is the ordinary structure factor and

$$(7.13)\quad \sigma(k,\omega) = (\frac{c_p - c_v}{c_p})\frac{2\lambda k^2/\rho_0 c_p}{(\lambda k^2/\rho_0 c_p)^2 + \omega^2}$$

$$+ \frac{c_v}{c_p}[\frac{\Gamma k^2}{(\Gamma k^2)^2 + (\omega + c_0 k)^2} + \frac{\Gamma k^2}{(\Gamma k^2)^2 + (\omega - c_0 k)^2}]\ .$$

B. Thermodynamic Aspects of Light Scattering

The significant parameters in the above $\sigma(k,\omega)$ can also be determined by quite direct thermodynamic arguments. Inasmuch as the scattering of light is directly due to density fluctuations (the index of refraction being a function of the density alone) and the variation of density is due both to a variation of the pressure and of the temperature (or entropy), the light scattered in a given direction owing to the density waves must consist of two parts: a mechanical [22] one with an altered frequency and a thermal part which must have the same frequency as the incident light. The basic ideas of this theory of light scattering go back to the work of Landau and Placzek who showed it to be especially appropriate to the case of liquid bodies where the entropy fluctuations are much larger than in solids. The frequency of the light scattered by the fluctuations at constant entropy (i.e. phonons) is shifted by an amount proportional to the velocity of the phonons. Energy and momentum considerations require that the proportionality constant be the magnitude of the change in the wave vector of the scattered light. Two lines are observed because scattering can occur from waves traveling in opposite directions but at the same speed. These lines are broadened somewhat because of the dissipative processes which damp out the waves. These lines are known as the Mandelshtam-Brillouin doublet.

The ratio of the intensity of this unshifted line I_0 to that of the two shifted components I_1 must be equal to the ratio between the square of the thermal part of the density fluctuation $\Delta\rho = (\partial\rho/\partial T)_p\ \Delta T$ or $\Delta\rho = (\partial\rho/\partial s)_p\ \Delta s$ and the square of its mechanical part $\Delta\rho = (\partial\rho/\partial p)_T\ \Delta p$ or $\Delta\rho=(\frac{\partial\rho}{\partial p})_s\ \Delta p$.

Following the method of Landau and Placzek the pressure and the specific entropy are chosen as independent variables (which is a reasonable choice for relatively long waves capable of effectively scattering light) and the volume V of a given small mass of the body as the dependent variable, in place of the entropy. Then one will have

$$(7.14) \qquad (\Delta V)_{S=\text{const.}} = \left(\frac{\partial V}{\partial p}\right)_S \Delta p = -\frac{V_0}{K_S}\Delta p$$

where K_S is the adiabatic bulk modulus and

$$(7.15) \qquad (\Delta V)_{p=\text{const.}} = \left(\frac{\partial V}{\partial S}\right)_p \Delta S = \left(\frac{\partial T}{\partial P}\right)_S \Delta S$$

the latter relation following from the differential expression for the total heat

$$(7.16) \qquad dJ = T\,dS + V\,dp\ .$$

Denoting the minimum value of the latter for the entire system (including the incremental volume portion) by J_0 we have further

$$(7.17) \quad -(\Delta J)_S \approx \frac{1}{2}\frac{\partial^2 J}{\partial \rho^2}(\Delta p)^2 = -\frac{1}{2}\left(\frac{\partial V}{\partial \rho}\right)_S(\Delta p)^2 = \frac{1}{2}VK_S(\Delta p)^2\ ,$$

and

$$(7.18) \quad -(\Delta J)_p \approx \frac{1}{2}\frac{\partial^2 J}{\partial S^2}(\Delta S)^2 = \frac{1}{2}\left(\frac{\partial T}{\partial S}\right)_p(\Delta S)^2 = \frac{T}{2c_p}(\Delta S)^2\ .$$

Therefore it follows that

$$(7.19) \quad \overline{(\Delta p)^2} = \frac{\int_{-\infty}^{\infty}(\Delta p)^2\, e^{-(\Delta T)_S/kT}\, d(\Delta p)}{\int_{-\infty}^{\infty} e^{-(\Delta J)_S/kT}\, d(\Delta p)} = \frac{-\,kT}{\left(\frac{\partial V}{\partial p}\right)} = \frac{kT}{V}K_S$$

and

$$(7.20)\quad \overline{(\Delta S)^2} = \frac{\int_{-\infty}^{\infty} (\Delta S)^2 \, e^{-(\Delta J)_p/kT} \, d(\Delta S)}{\int_{-\infty}^{\infty} (e^{-(\Delta J)_p/kT} \, d(\Delta S)} = \frac{kT}{(\frac{\partial T}{\partial S})_p} = c_p k$$

Thus,

$$(7.21)\qquad I_0/I_1 = (\frac{\partial V}{\partial S})_p^2 \overline{(\Delta S)^2} \;/\; (\frac{\partial V}{\partial p})_S^2 \overline{(\Delta p)^2} \;,$$

and using the identities

$$(\frac{\partial V}{\partial S})_p / (\frac{\partial V}{\partial p})_S = -\,(\frac{\partial p}{\partial S})_V \quad \text{and} \quad (\frac{\partial T}{\partial p})_S / (\frac{\partial T}{\partial S})_p = -\,(\frac{\partial S}{\partial p})_T$$

and the thermodynamic relation $(\partial V/\partial S)_p = (\partial T/\partial p)_S$ the ratio can be rewritten

$$(7.22)\qquad I_0/I_1 = (\frac{\partial p}{\partial S})_V (\frac{\partial S}{\partial p})_T \;.$$

Moreover,

$$(\frac{\partial p}{\partial V})_T = (\frac{\partial p}{\partial V})_S + (\frac{\partial p}{\partial S})_V (\frac{\partial S}{\partial V})_T$$

so

$$(7.23)\quad \frac{I_0}{I_1} = [(\frac{\partial p}{\partial V})_T - (\frac{\partial p}{\partial V})_S] \frac{(\frac{\partial S}{\partial p})_T}{(\frac{\partial S}{\partial V})_T} = \frac{(\frac{\partial p}{\partial V})_T - (\frac{\partial p}{\partial V})_S}{(\frac{\partial p}{\partial V})_T} = \frac{K_S - K_T}{K_T} = \frac{c_p - c_v}{c_v}$$

where $K_T = -V(\partial p/\partial V)_T$ is the isothermal bulk modulus and c_p and c_v are the specific heats at constant pressure and constant volume.

Landau and Placzek have observed that the widths of these lines is determined by the lifetimes of the density fluctuations which can be described by the linearized hydrodynamic equations of irreversible thermodynamics.

There have been numerous attempts to observe the spectrum of the light scattered by density fluctuations. It has been possible to detect the presence of Brillouin lines in liquids using the techniques of high resolution spectroscopy.

It can be shown, by adapting Van Hove's neutron-scattering results to light scattering, that the intensity I' of light scattered from a fluid is

$$I'(\underset{\sim}{R},\omega) = \frac{\alpha^2\Omega^4 N}{2\pi c^4 R^2} I_0 \sin^2\phi \; s(\underset{\sim}{k},\omega) \; . \tag{7.24}$$

The light, scattered at the origin, is observed at $\underset{\sim}{R}$. The angular frequency of the scattered light is Ω, ω is the shift in the angular frequency and $\underset{\sim}{k}$ is the change in the wave vector of the scattered light from that of the incident light in the medium $\underset{\sim}{k}_1$; $k=k_1 2\sin(\theta/2)$, where θ is the scattering angle. There are N spherically symmetric molecules of polarizability α in the scattering volume. The incident light is assumed to be in the form of a plane polarized monochromatic wave. The angle between $\underset{\sim}{R}$ and the electric vector of the incident wave is denoted by ϕ. The polarization of the scattered light depends only on ϕ because the molecules are isotropic.

Thus it is seen possible to study the spectral distribution of light scattered by density fluctuations. Moreover, a way is now available to measure transport properties of the fluid without the imposition of a gradient as for instance the bulk viscosity can be inferred from width† of Brillouin lines.

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†The width of the central line is proportional to the thermal diffusivity, $\lambda/\rho_0 c_p$. Interest in this quantity is greatest near the critical point where conventional measurements of the thermal conductivity are difficult.

Appendix A: Crystal Lattice of Coupled Oscillators

The basic Hamiltonian is

$$(A.1) \qquad H = \frac{1}{2m} \sum_{j=1}^{N} p_j^2 + \sum_{i,j} \frac{1}{2} q_j A_{jk} q_k \ .$$

The A_{jk} matrix depends upon the force constants. By transforming to normal coordinates $\{P_k\}$ and $\{Q_k\}$ via

$$(A.2) \qquad p_j = \sum_k c_{jk} P_k \ ; \qquad q_j = \sum_k c_{jk} Q_k$$

one obtains a new Hamiltonian

$$(A.3) \qquad H = \frac{1}{2} \sum_{j=1}^{N} \left(\frac{1}{m} P_j^2 + m\omega_j^2 Q_j^2\right)$$

where ω_j is the j-th normal mode frequency and the matrix c_{jk} satisfies

$$(A.4) \qquad \sum_j c_{jk} c_{j\ell}^* = \delta_{k\ell} \ .$$

The variation of the normal mode Q_k's and P_k's with time follows from

$$m \ddot{Q}_k + \omega_k^2 Q_k = 0 \ ;$$

as expected one finds

$$(A.5) \qquad Q_k(t) = \frac{P_k(0)}{m\omega_k} \sin \omega_k t + Q_k(0) \cos \omega_k t$$

$$P_k(t) = P_k(0) \cos \omega_k t - m\omega_k Q_k(0) \sin \omega_k t \ .$$

The momentum of the j-th particle at time t is:

$$p_j(t) = \sum_k a_{jk} p_k(0) + \sum_k b_{jk} Q_k(0)$$

where

$$(A.6) \qquad a_{jk} = \sum_s c_{js} c_{ks}^* \cos \omega_s t; \quad b_{jk} = -c_{jk} m\omega_k \sin \omega_k t.$$

From orthogonality one has

$$\sum_j a_{jj} = \sum_k \cos \omega_k t.$$

Also

(A.7) $$\sum_k (a_{jk}^2+(m\omega_k)^{-2}b_{jk}^2) = 1.$$

In an n-dimensional cubic lattice the c_{jk}'s are

(A.8) $$c_{jk} = M^{-n/2} \exp 2\pi i(\sum_{\alpha=1}^{n} j_\alpha k_\alpha)/M$$

where j and k are vectors with components $\{j_\alpha\}$ and $\{k_\alpha\}$ each k,j runs through integers

$$j_\alpha = 1,2,3,\ldots,M; \quad k_\alpha = 1,2,3,\ldots,M.$$

If n = 1 (linear lattice)

(A.9) $$c_{jk} = M^{-1/2}\exp 2\pi i \frac{j_\alpha k_\alpha}{M} = M^{-1/2} \exp 2\pi i \frac{j_1 k_1}{M}$$

$$j_1 = 1,2,3,\ldots,M; \quad k_1 = 1,2,3,\ldots,M$$

and orthogonality becomes

(A.10) $$\sum_{j_1} M^{-1/2} \exp 2\pi i \frac{j_1 k_1}{M} \cdot M^{-1/2} \exp -2\pi i \frac{j_1 \ell_1}{M} = \delta_{k_1 \ell_1}.$$

Therefore

(A.11) $$p_{j_1} = \sum_{k_1} \frac{1}{\sqrt{M}} e^{2\pi i j_1 k_1/M} P_{k_1}; \quad q_{j_1} = \sum_{k_1} \frac{1}{\sqrt{M}} e^{2\pi i j_1 k_1/M} Q_{k_1}.$$

In addition one has [21]

(A.12) $$\sum_{k,\ell} \frac{A_{k\ell}}{M} e^{2\pi i n\ell/M} e^{-2\pi i nk/M} = m\omega_n^2 .$$

Moreover the transformation is unitary since

(A.13) $$\sum_{j_1} q_{j_1} q_{j_1}^* = \sum_{j_1,k_1,k_2} \frac{1}{\sqrt{M}} e^{2\pi i j_1 k_1/M} Q_{k_1} \frac{1}{M} e^{-2\pi i j_1 k_2/M} Q_{k_2}^*$$

$$= \sum_{k_1,k_2} \delta_{k_1 k_2} Q_{k_1} Q_{k_2}^* = \sum_{k_1} Q_{k_1} Q_{k_1}^* ,$$

and finally since k_1 was a dummy index,

$$\sum_{j_1} (q_{j_1} q^*_{j_1} - Q_{j_1} Q^*_{j_1}) = 0 \ .$$

In addition the normal mode frequencies of an $N = M^n$, n-dimensional nearest neighbor lattice are to be used and are

$$\text{(A.14)} \quad m\omega^2 = 4 \sum_{j=1}^{n} \gamma_j \sin^2 \frac{\pi k_j}{M} \ ; \quad k_j = 1,2,3,\ldots,M,$$

where γ is the force constant in various directions and m is the mass of each particle. The frequency spectrum for a linear lattice is

$$\text{(A.15)} \qquad g(\omega) = \frac{2}{\pi} (\omega_L^2 - \omega^2)^{-1/2}$$

$$m\omega_L^2 = 4\gamma_1$$

$$m\omega^2 = 4\gamma_1 \sin^2 \frac{\pi k_1}{M} \qquad \text{as } N \to \infty$$

Here $g(\omega)\, d\omega$ is the fraction of frequencies between ω and $\omega + d\omega$ while ω_L is the largest frequency.

Appendix B: Explicit Integration of Initial Velocity Dependence.

Integrating out $\dot{x}_j(0)$ from $\int \lambda(\bar{B}-B+1)e^{-\bar{B}}\ldots$ can be accomplished before transforming to normal modes. Here, the relevant part of the kernel is

$$\int_{-\infty}^{\infty} d\dot{x}_j(0)\, e^{-\frac{1}{2} r \sum_j \dot{x}_j(t)\dot{x}_j(0)}\, e^{-\frac{1}{2} \sum_j m\beta \dot{x}_j^2(0)} \cdot e^{-i \int_0^t \sum_j \xi_j(t')\dot{x}_j(0)dt'} . \tag{B.1}$$

Expressed in vector notation [23] (B.1) is

$$\int_{-\infty}^{\infty} d\dot{\underset{\sim}{x}}(0)\, e^{-\frac{1}{2} r\dot{\underset{\sim}{x}}(t)\cdot\dot{\underset{\sim}{x}}(0)}\, e^{-\frac{1}{2} m\beta\dot{\underset{\sim}{x}}(0)\cdot\dot{\underset{\sim}{x}}(0)} \cdot e^{-i\int_0^t \underset{\sim}{\xi}(t')\cdot\dot{\underset{\sim}{x}}(0)dt} ; \tag{B.2}$$

integrating,

$$\left(\frac{2\pi}{m\beta}\right)^{1/2} \exp - \frac{1}{2m\beta} \left[\int_0^t \int_0^{t'} \underset{\sim}{\xi}(t')\cdot\underset{\sim}{\xi}(t'')\, dt'\, dt'' - ir\int_0^t \dot{\underset{\sim}{x}}(t)\cdot\underset{\sim}{\xi}(t')\, dt' - \frac{1}{4} r^2 \dot{\underset{\sim}{x}}(t)\cdot\dot{\underset{\sim}{x}}(t)\right] \tag{B.3}$$

for which explicit use of the formula

$$\int \ldots \int e^{-\frac{1}{2}\sum y_\alpha c_{\alpha\beta} y_\beta}\, e^{i\sum D_\alpha y_\alpha} \prod dy_\alpha = (\sqrt{2\pi})^n (\mathrm{Det}\ \ C)^{-1/2}\, e^{-\frac{1}{2}\sum D_\alpha (c^{-1})_{\alpha\beta} D_\beta}$$

was made.

Appendix C: N-Body Variational Equations

The N-body kernel under the normal mode transformation is

$$(\text{C.1})\quad \exp -\frac{1}{2m\beta}\sum_k \Big[\int_0^t\int_0^{t'} \xi(k,t')\xi(-k,t'')\,dt'\,dt'' - ir\int_0^t \dot{x}(k,t)\xi(-k,t')dt' - \frac{1}{4}r^2\dot{x}(k,t)\dot{x}(-k,t)\Big]$$

$$\cdot\, e^{-m\beta\sum_k e^{\pm 2\pi ik/M}\,\omega^2 x(k,0)x(-k,0)}$$

$$\cdot\, e^{i\sum_k\int_0^t \xi(k,t')\dot{x}(-k,t')dt'}$$

$$\cdot\, e^{\frac{i}{m}\sum_k\int_0^t\int_0^{t'} m\omega^2\xi(k,t')x(-k,t'')dt'\,dt''}$$

subject to $\omega = 2(\gamma/m)^{1/2}\sin \pi k/M$.

The variation of the kernel is made by taking $\delta/\delta\xi(\underset{\sim}{k},\tau)$ and $\delta/\delta x(\underset{\sim}{k},\tau)$ with $\tau = t', t''$ and $\underset{\sim}{k} = \pm k$ (since the kernel is symmetric in k). This gives

$$(\text{C.2})\quad \sum_{\underset{\sim}{k}}\Big(-\frac{1}{m\beta}\int_0^t \xi(\underset{\sim}{k},t')\,dt' + \frac{ir}{2m\beta}\dot{x}(\underset{\sim}{k},t) + i\dot{x}(\underset{\sim}{k},\tau) + i\int_0^\tau \omega^2 x(\underset{\sim}{k},t'')\,dt''\Big) = 0$$

$$\sum_{\underset{\sim}{k}}\Big(-i\dot{\xi}(\underset{\sim}{k},\tau) + i\int_\tau^t \omega^2\xi(\underset{\sim}{k},t')dt'\Big) = 0\ .$$

τ-differentiating (C.2) yields

$$(\text{C.3})\quad \sum_k (\ddot{x}(\underset{\sim}{k},\tau) - \omega^2 x(\underset{\sim}{k},\tau) = 0\ ;\quad \sum_{\underset{\sim}{k}}(\ddot{\xi}(\underset{\sim}{k},\tau) - \omega^2\xi(\underset{\sim}{k},\tau)) = 0;$$

and putting (C.3) back into (C.2) gives

$$(C.3)' \quad \sum_{\underset{\sim}{k}} (\dot{\xi}(\underset{\sim}{k},\tau) + \int_{\tau}^{t} \omega^2 \xi(\underset{\sim}{k},t')dt') = 0$$

$$\sum_{\underset{\sim}{k}} (\dot{\xi}(\underset{\sim}{k},\tau) + \int_{\tau}^{t} \ddot{\xi}(\underset{\sim}{k},t')\, dt') = 0$$

which reduces to

$$(C.4) \quad \sum_{\underset{\sim}{k}} \dot{\xi}(\underset{\sim}{k},t) = 0 \text{ , a boundary condition.}$$

In like manner,

$$(C.5) \quad \sum_{\underset{\sim}{k}} (- \frac{1}{m\beta} \int_{0}^{t} \frac{1}{\omega^2} \ddot{\xi}(\underset{\sim}{k},t')dt' + \frac{ir}{2m\beta} \dot{x}(\underset{\sim}{k},t) + i\dot{x}(\underset{\sim}{k},\tau) - i \int_{0}^{\tau} \ddot{x}(\underset{\sim}{k},t'')\, dt'') = 0$$

implies

$$(C.6) \quad \sum_{\underset{\sim}{k}} \dot{\xi}(\underset{\sim}{k},0) = \sum_{\underset{\sim}{k}} \frac{1}{2} ir\omega^2 \dot{x}(\underset{\sim}{k},t) + im\beta\omega^2 \dot{x}(\underset{\sim}{k},0)$$

which is a coupling condition. The differential equation set (C.3) when solved subject to (C.4) and (C.5) and the tautology $x(\underset{\sim}{k},0) = x(\underset{\sim}{k},0)$, $x(\underset{\sim}{k},t) = x(\underset{\sim}{k},t)$ gives, as expected, the solution

$$(C.7) \quad x(\underset{\sim}{k},\tau) = \frac{x(\underset{\sim}{k},t) \sin \omega\tau + x(\underset{\sim}{k},0) \sin \omega(t-\tau)}{\sin \omega\tau}$$

$$(C.8) \quad \xi(\underset{\sim}{k},\tau) = i\beta m\omega^2 (\frac{x(\underset{\sim}{k},t) - x(\underset{\sim}{k},0)\cos \omega t}{\sin^2 \omega t}) \cos \omega(t-\tau)$$

$$+ \frac{1}{2} ir\omega^2 (\frac{x(\underset{\sim}{k},t)\cos \omega t - x(\underset{\sim}{k},0)}{\sin^2 \omega t}) \cos \omega(t-\tau).$$

If equations (C.7) and (C.8) are now reintroduced into expression (C.1) it becomes after algebraic manipulation[†]

$$(\text{C.9})\quad e^{-m\beta\sum_{\underset{\sim}{k}} e^{2\pi i\underset{\sim}{k}/M}\,\omega^2 x^2(\underset{\sim}{k},0)}\; e^{ir/4m\beta \sum_{\underset{\sim}{k}} \dot{x}(\underset{\sim}{k},t)\int_0^t \xi(\underset{\sim}{k},t')dt'}$$

$$\cdot\; e^{-\frac{1}{2m\beta}\left(\sum_{\underset{\sim}{k}} - \frac{1}{4} r^2 \dot{x}^2(\underset{\sim}{k},t)\right)}\; e^{\frac{1}{2} i \sum_{\underset{\sim}{k}}(\xi(\underset{\sim}{k},t)x(\underset{\sim}{k},t)-\xi(\underset{\sim}{k},0)x(\underset{\sim}{k},0))}$$

which after further arrangement is expressible as

$$\exp - \frac{1}{2}\sum_{k} (c_{11}(k)x^2(k,0)+ 2c_{12}(k)x(k,0)x(k,t)+ c_{22}(k)x^2(k,t))$$

with

$$c_{11}(k) = \beta m\omega^2\, e^{2\pi ik/M} + \frac{\beta m\omega^2\cos^2\omega t}{\sin^2\omega t} + \frac{r\omega^2\,\cos\,\omega t}{\sin^2\omega t}$$

$$c_{22}(k) = \frac{\beta m\omega^2}{\sin^2\omega t} + \frac{r\omega^2\,\cos\,\omega t}{\sin^2\omega t}$$

$$c_{12}(k) = -\,\frac{\beta m\omega^2\,\cos\,\omega t}{\sin^2\omega t} - \frac{1}{2}\, r\omega^2\left(\frac{1+\cos^2\omega t}{\sin^2\omega t}\right)$$

[†] See Chapter II, equations (2.11)-(2.14) for an analogous calculation.

Appendix D.

I. Typical Multiple Integrals of N-Body Calculation.

In carrying out the evaluation of the three third order integrals containing $e^{\gamma t''}\xi(t')x^3(t'')$ the following typical forms arise (for which terms linear in γ are immediately dropped since as $\gamma \to 0$ they contribute zero).

$$\text{(DI.1)} \quad \int_{-\infty}^{0}\int_{-\infty}^{t'} e^{\gamma t''} \sin^3\omega t'' \cos\omega(t-t')\,dt'\,dt''$$

$$= \int_{-\infty}^{0} \frac{e^{\gamma t'}\cos\omega(t-t')}{\gamma^2+9\omega^2}[\gamma\sin^3\omega t' - 3\omega\sin^2\omega t'\cos\omega t'$$

$$+ \frac{6\omega^2}{\gamma^2+\omega^2}(\gamma\sin\omega t' - \omega\cos\omega t')]\,dt'$$

$$\to -\frac{1}{3\omega}\left[\frac{\cos\omega t}{8\gamma} - \frac{\omega\sin\omega t}{8\omega^2} + \frac{\omega\sin\omega t}{32\omega^2} - \frac{\cos\omega t}{\gamma} + \frac{\sin\omega t}{2\omega}\right]$$

$$\text{(DI.2)} \quad \int_{0}^{t}\int_{-\infty}^{0} e^{\gamma t''} \sin^3\omega t'' \cos\omega(t-t')\,dt'\,dt''$$

$$= \int_{0}^{t} \frac{-6\omega^3}{(\gamma^2+9\omega^2)(\gamma^2+\omega^2)}\cos\omega(t-t')\,dt' \to -\frac{2}{3\omega^2}\sin\omega t.$$

II. Representative Quadratic Square Forms.

In the explicit evaluation of inequality (6.30) one encounters such integrals as

$$\text{(DII.1)}\quad \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{1}{2}(2c_{12}(k)x(k,0)x(k,t)+c_{22}(k)x^2(k,t))}$$

$$\cdot\ e^{-\frac{1}{2}(c_{11}(k)x^2(k,0)}\quad x(k,t)x^3(k,0)\ dx(k,0)\ dx(k,t))$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} x(k,t)x^3(k,0)\ e^{-\frac{1}{2}c_{22}(k)[x(k,t)+\frac{c_{12}(k)}{c_{22}(k)}x(k,0)]^2}$$

$$\cdot\ e^{-\frac{1}{2}c_{11}(k)x^2(k,0)}\ e^{\frac{1}{2}\frac{c_{12}^2(k)}{c_{22}(k)}x^2(k,0)}\quad dx(k,0)\ dx(k,t)$$

Let $v = x(k,t) + \frac{c_{12}(k)}{c_{22}(k)}x(k,0)$ then the integral becomes

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} (vx^3(k,0) - \frac{c_{12}(k)}{c_{22}(k)}x^4(k,0))\ e^{-\frac{1}{2}c_{22}(k)v^2}$$

$$\cdot\ e^{-\frac{1}{2}[c_{11}(k)-\frac{c_{12}^2(k)}{c_{22}(k)}]x^2(k,0)}\quad dv\ dx(k,0)$$

$$= \ -3\pi c_{12}(k)c_{22}(k)\ /\ 2(c_{11}(k)c_{22}(k)-c_{12}^2(k))^{5/2}$$

$$\text{(DII.2)}\quad \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{1}{2}(2c_{12}(k)x(k,0)x(k,t)+c_{11}(k)x^2(k,0))}$$

$$\cdot\ e^{-\frac{1}{2}c_{22}(k)x^2(k,t)}\quad x(k,0)x^3(k,t)\ dx(k,0)\ dx(k,t)$$

$$= \frac{-3\pi\ c_{12}(k)\ c_{11}(k)}{2(c_{11}(k)c_{22}(k)-c_{12}^2(k))^{5/2}}$$ by the symmetric exchange

of $c_{22}(k)$ for $c_{11}(k)$. The recurrent denominator explicitly is

$$(c_{11}(k)c_{22}(k)-c_{12}^2(k))\Big|_{t\to i\tau} = (\beta m\omega^2 e^{2\pi ik/M} - \beta m\omega^2\,\frac{\cosh\,\omega\tau}{\sinh^2\omega\tau}\ -$$

$$- r\omega^2 \frac{\cosh \omega\tau}{\sinh^2 \omega\tau})(- \frac{\beta m\omega^2}{\sinh^2 \omega\tau} - r\omega^2 \frac{\cosh \omega\tau}{\sinh^2 \omega\tau})$$

$$- (-\beta m\omega^2 \frac{\cosh \omega\tau}{\sinh^2 \omega\tau} - \frac{r\omega(1+\cosh^2 \omega\tau)}{2 \sinh^2 \omega\tau})^2$$

and

$$(c_{11}(k)c_{22}(k) - c_{12}^2(k))\Big|_{\substack{t\to i\tau \\ r=0}} = \frac{\beta^2 m^2 \omega^4}{\sinh^2 \omega\tau}(-e^{2\pi ik/M}$$

$$+ \frac{\cosh \omega\tau}{\sinh^2 \omega\tau} - \frac{\cosh^2 \omega\tau}{\sinh^2 \omega\tau}) .$$

Also one needs

$$\frac{\partial}{\partial r} (c_{11}(k)c_{22}(k) - c_{12}^2(k))^{-n/2}\Big|_{\substack{r=0 \\ t\to i\tau}} \qquad \text{for } n = 1,3,5,\ldots$$

$$= \frac{-n/2}{(c_{11}(k)c_{22}(k)-c_{12}^2(k))^{(n+2)/2}} \frac{\partial}{\partial r}(c_{11}(k)c_{22}(k)-c_{12}^2(k))\Big|_{\substack{r=0 \\ t\to i\tau}}$$

$$= \frac{- \frac{n}{2} \frac{\beta m\omega^4 \cosh \omega\tau}{\sinh^2 \omega\tau}(-e^{2\pi ik/M} + \frac{\cosh \omega\tau}{\sinh^2 \omega\tau} - \frac{\cosh^2 \omega\tau}{\sinh^2 \omega\tau})}{[\frac{\beta^2 m^2 \omega^4}{\sinh^2 \omega\tau} (-e^{2\pi ik/M} + \frac{\cosh \omega\tau}{\sinh^2 \omega\tau} - \frac{\cosh^2 \omega\tau}{\sinh^2 \omega\tau})]^{(n+2)/2}}$$

III. N-Body Renormalization by Way of Square of Frequency Shift.

As mentioned in Chapter VI, the renormalization procedure for expression (6.30) is carried out about the square of the frequency shift. Typically, one has

$$\text{(DIII.1)}\quad \ldots m\beta(x(k,t)x(-k,t)-x(k,0)x(-k,t)\cos\omega t)$$

$$\cdot\psi(s,j,k,\ldots)(b_1(t)+1)+\ldots = [\Omega^2(e^{\pm 2\pi ik/M}-1)$$

$$\cdot\ (m\beta(x(k,t)x(-k,t)-x(k,0)x(-k,t)\cos\omega t)c_1(t)$$

$$+\ m\beta(x(k,t)x(-k,0)\ -\ x(k,0)x(-k,0)\cos\omega t)c_2(t))]^2$$

After rearrangement,

$$\text{(DIII.2)}\quad \Omega^4 = \{\ldots m\beta(x(k,t)x(-k,t)-x(k,0)x(-k,t)\cos\omega t)$$

$$\cdot\psi(s,j,k,\ldots)\left(\frac{\sin\omega t}{2\omega}-\frac{t\cos\omega t}{2}+\ldots\right\}\ /\ \{[(e^{\pm 2\pi ik/M}-1)$$

$$\cdot(m\beta(x(k,t)x(-k,t)-x(k,0)x(-k,t)\cos\omega t)(-\tfrac{1}{2}\,t\cos\omega t)$$

$$+\ m\beta(x(k,t)x(-k,0)-x(k,0)x(-k,0)\cos\omega t)(\tfrac{1}{2}\,t-\tfrac{1}{2}\,t\cos\omega t)]^2$$

$$+\ \text{linear terms} + \text{oscillating terms}\}.$$

Now the numerator either oscillates or linearly goes to infinity while the denominator quadratically goes to infinity and thus $\Omega^2 \to 0$ as $t \to \infty$. A second characteristic form to be examined is

$$\text{(DIII.3)}\quad \ldots[x(k,0)x(-k',t)x(-k'',t)x(-k''',t)]$$

$$\cdot\left[a_5(t)-\frac{3\beta\omega\cos^2\omega t}{8\gamma\sin^5\omega t}\right]\Bigg|_{r=0} +\ldots = [\Omega^2(e^{\pm 2\pi ik/M}-1)\cdot$$

$$\cdot(m\beta(x(k,t)x(-k,t)-x(k,0)x(-k,t)\cos\omega t)c_1(t)\ +$$

$$+ m\beta(x(k,t)x(-k,0)-x(k,0)x(-k,0)\cos \omega t)\ c_2(t)]^2$$

where all the $a_i(t)$ terms containing a $1/\gamma$ contribution have correspondingly been cancelled in pairs (e.g. $a_1 \to a_6$, $a_2 \to a_5$, $a_4 \to a_7$, $a_3 \to a_8$) before letting $\gamma \to 0$ because all are structured alike[†] viz. each has a coefficient like $x(k,0)x(-k,t)x(-k'',t)x(-k''',t)$ which is just a fourth power of position times a $\beta\omega \cos \omega t/\sin^5\omega t$ or $\beta\omega/\sin^5\omega t$. Hence after algebra and direct substitution for $c_1(t)$, $c_2(t)$ and $a_5(t)$,

$$\text{(DIII.4)}\quad \Omega^4 = \ldots[x(k,0)x(-k',t)x(-k'',t)x(-k''',t)]$$

$$\cdot[\beta \cos \omega t(\frac{\sin 4\omega t \cos \omega t}{96} + \frac{5 \sin \omega t \cos 2\omega t}{24}$$

$$- \frac{\sin \omega t \cos 4\omega t}{96} - \frac{\cos \omega t \sin 2\omega t}{6})]+\ldots$$

$$/ \sin^5\omega t[m\beta x(k,t)x(-k,t)-x(k,0)x(-k,t) \cos \omega t)$$

$$\cdot(\frac{1}{2\omega} \sin \omega t-\frac{1}{2}\ t \cos \omega t)+ m\beta(x(k,t)x(-k,0)-x(k,0)$$

$$\cdot x(-k,0) \cos \omega t)(\frac{1}{4\omega} \sin 2\omega t - \frac{1}{2\omega} \sin \omega t+ \frac{1}{2}\ t - \frac{1}{2}\ t \cos \omega t)]^2$$

It is convenient to make the complex extension at this point and so one may consider as typical

$$\text{(DIII.5)}\quad \ldots \sinh 4\omega\tau \cosh^2\omega\tau/\ldots\sinh^5\omega\tau(\frac{1}{\omega} \sinh \omega\tau-\tau \cosh \omega\tau)$$

which in the infinite time limit goes to zero and once again Ω^2 is zero.

[†] If one lets $t \to i\tau$ and then $\tau \to \infty$ their orders balance.

Appendix E: Path Integral Linear Terms.

For linear terms in the functional integral one has the expression

$$\int_{-\infty}^{\infty}\cdots\int \underset{\sim}{y}\, e^{-(y^{T}Ay+\underset{\sim}{B}\cdot\underset{\sim}{y})}\, dy \ldots \quad .$$

To integrate such terms one solves

$$2\, Ay + B = 0$$

$$y = -\tfrac{1}{2} A^{-1}B \equiv y^{0} = y_{\text{stationary}}$$

Let $y' = y + \frac{1}{2} A^{-1}B$ and therefore

$$\int_{-\infty}^{\infty}\cdots\int (y' - \tfrac{1}{2} A^{-1}B) e^{-(y'^{T}Ay')}\, e^{-\frac{1}{4} B\cdot A^{-1}B}\, dy' \ldots$$

$$= y^{0} \int \ldots \int e^{-y'^{T}Ay'}\, e^{-\frac{1}{4} B\cdot A^{-1}B}\, dy' \ldots ,$$

since y' is an odd function.

Appendix F: The Reduced Quartic Equation.

The quartic equation [27]

$$y^4 + py^3 + hy^2 + ry + s = 0$$

may be reduced to the form

$$z^4 + \alpha z^2 + \beta z + \gamma = 0$$

by the substitution $y = (z - P/4)$. Let ℓ, m, n denote the roots of the resolvent cubic $t^3 + (\frac{1}{2}\alpha)t^2 + (\frac{\alpha^2 - 4\gamma}{16})t - \frac{1}{64}\beta^2 = 0$. The roots of the reduced quartic are

$$z_1 = \pm(-\sqrt{\ell} - \sqrt{m} - \sqrt{n}) \ ; \quad z_2 = \pm(-\sqrt{\ell} + \sqrt{m} + \sqrt{n})$$

(F.1)

$$z_3 = \pm(\sqrt{\ell} - \sqrt{m} + \sqrt{n}) \ ; \quad z_4 = \pm(\sqrt{\ell} + \sqrt{m} - \sqrt{n})$$

where the upper sign is used if β is positive and the lower sign if β is negative. Therefore, if we let

$$c = z - \frac{1}{2}q \quad \text{with} \quad p = 2q \ ; \quad h = -1$$

$$s = q \ , \quad \text{and} \quad r = -2q \ ,$$

we have

$$(z - \frac{1}{2}q)^4 + 2q(z - \frac{1}{2}q)^3 - (z - \frac{1}{2}q)^2 - 2q(z - \frac{1}{2}q) + q = 0$$

$$= z^4 - (1 + \frac{3}{2}q^2)z^2 + (q^3 - q)z + (-\frac{3}{16}q^4 + \frac{3}{4}q^2 + q) = 0$$

with $\alpha = -(1 + \frac{3}{2}q^2)$; $\beta = q^3 - q$; $\gamma = -\frac{3}{16}q^4 + \frac{3}{4}q^2 + q$.

The cubic equation $t^3 + a_1t^2 + a_2t + a_3 = 0$ may be reduced by the substitution $t = (w - a_1/3)$ to the normal form $w^3 + \delta w + \theta = 0$ for which $\delta = \frac{1}{3}(3a_2 - a_1^2)$; $\theta = \frac{1}{27}(3a_1^3 - 9a_1a_2 + 27a_3)$ with solutions ℓ, m, n. ($\ell = A + B$; $m, n = \frac{-(A+B)}{2} \pm \frac{i\sqrt{3}}{2}(A - B)$; $A, B = [-\frac{1}{2}\theta \pm \sqrt{\theta^2/4 + \delta^3/27}\ ]^{1/3}$).

For our case we have $a_1 = \frac{1}{2}\alpha$; $a_2 = \frac{\alpha^2-4\gamma}{16}$; $a_3 = -\frac{\beta^2}{64}$ and

$$A,B = \Big[-\frac{1}{54}\Big(\frac{3\alpha^3}{8} + \frac{9\alpha\beta^2}{128} - \frac{27}{64}\beta^2\Big) + \Big\{\frac{1}{4}\Big[\frac{1}{27}\Big(\frac{3\alpha^2}{8} + \frac{9\alpha\beta^2}{128}$$

$$- \frac{27}{64}\beta^2\Big)\Big]^2 + \frac{1}{27}\Big[\frac{\alpha^2-4\gamma}{16} - \frac{\alpha^2}{12}\Big]^3\Big\}^{1/2}\Big]^{1/3}.$$

If $\theta^2/4 + \delta^3/27 > 0$, then there are one real root and two conjugate imaginary roots for the cubic, where

$$\frac{\theta^2}{4} + \frac{\delta^3}{27} = \frac{1}{4(27)^2}\Big[\frac{9\alpha^6}{64} + \frac{81\alpha^2\beta^4}{(128)^2} + \Big(\frac{27}{64}\Big)^2\beta^4 + \frac{27}{(8)(64)}\alpha^4\beta^2$$

$$- \frac{3(27)}{(8)(32)}\alpha^3\beta^2 - \frac{9(27)}{(64)^2}\alpha\beta^4\Big] - \frac{1}{27}\Big[\frac{\alpha^6}{(48)^3} + \frac{3\alpha^4\gamma}{4(48)^2} + \frac{3\alpha^2\gamma^2}{(16)(48)} + \frac{\gamma^3}{64}\Big]$$

Since $0 < q < 1$ it follows that

$$\alpha^3 = -\Big(1 + \frac{3}{2}q^2\Big)^3 < 0$$

$$\alpha\beta^2 = -\Big(1 + \frac{3}{2}q^2\Big)q^2(q-1)^2(q+1)^2 < 0$$

$$\beta^2 = q^2(q-1)^2(q+1)^2 > 0$$

$$\alpha^2 = \Big(1 + \frac{3}{2}q^2\Big)^2 > 0$$

$$\gamma = -\frac{3}{16}q^4 + \frac{3}{4}q^2 + q > 0 .$$

By examination of the discriminant near the end points of q (and at any intermediate value) it is indeed found to be positive definite. Thus, for

$$q \simeq \gamma \simeq 1 ; \quad \beta^4 \approx 0 ; \quad \alpha \simeq -2.5 ;$$

one finds the leading positive term of $\theta^2/4 + \delta^3/27$ to be

$$\frac{1}{27}\left(\frac{(2.5)^6}{(12)(64)}\right) = \frac{1}{27}\left(\frac{61}{100} + \ldots\right)$$

whereas all the combined negative terms are $-\frac{1}{27}\left(\frac{5}{100}\right)$ and therefore the discriminant is postiive definite. Likewise, for

$$q \mathrel{\widetilde{\sim}} \gamma << 1 \; ; \qquad \beta^4 \mathrel{\widetilde{\sim}} q^4 \; ; \qquad \alpha \simeq -1$$

one finds

$$\frac{1}{27}\left[\frac{1}{768} - \frac{1}{110{,}592} - \frac{q}{3072} + \ldots\right]$$

which is also positive definite. This implies that the roots of the quartic are complex (i.e. expression (F.1)), and hence the coefficient of the t term cannot reach zero for any real values of cos $\omega_0 t$.

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